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Risø Report No. 288

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Danish Atomic Energy Commission

Research Establishment Risø

Physics Department

Annual Progress Report

1 January – 31 December 1972

March 1973

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Danish Atomic Energy Commission
Research Establishment Risø

PHYSICS DEPARTMENT
ANNUAL PROGRESS REPORT

1. January - 31. December 1972

edited by
H. Bjerrum Møller and C. J. Christensen

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CONTENTS

SUMMARY

The research work in the Physics Department at Risø covers four main fields:

Solid-State Physics (Neutron Scattering)

Plasma Physics

Nuclear Spectroscopy

Meteorology

The principal activities in these fields are presented in this report covering the period from 1 January to 31 December 1972.

The solid-state physics section utilizes thermal neutron beams from the DR 3 reactor for experimental studies of solids and liquids. Six neutron spectrometers are available for these experiments: Three triple-axis, two double-axis, and one multiangle-reflecting crystal spectrometer with a position-sensitive detector (MARX spectrometer). An additional diffractometer is used for structural studies by the Institute of Chemistry, University of Aarhus. The liquid-hydrogen cold source is nearly ready for installation in the DR 3 reactor. Cold neutrons will presumably be available from the late summer of 1973. The construction of neutron-conducting tubes from the cold source to an experimental hall was started. We hope the tubes will be ready for installation in the spring of 1974.

The scientific investigations can be roughly classified as lying within the following fields: magnetism, lattice dynamics, liquids, and amorphous materials.

The neutron diffraction studies of the light rare earth metals were continued. The effect of applied magnetic fields up to 4.5 teslas (= 45 kgauss) on the magnetic structure of Nd was investigated and previous measurements of the magnetic form factor of Pr extended. In connection with these experiments, the magnetization of several light rare earth metals in high magnetic fields (up to 37 teslas) was measured in collaboration with the University of Amsterdam.

Studies of light rare earth compounds with a strong crystalline field were also continued. The exciton dispersion relation and various thermodynamical quantities were calculated for such systems by different field-theoretical methods. The exchange parameters were deduced for various rare earth pnictides by means of a general molecular field theory. Experimentally the crystal field splittings were studied in a number of compounds.

The anisotropic exchange interaction in the heavy rare earth metal Tb was further studied with measurements of the spin wave energies in higher magnetic fields (up to 10 teslas), and various corrections to the data were introduced. However, the measurements still indicate the existence of a strongly anisotropic exchange interaction. The conduction-electron susceptibility was calculated for rare earth metals in the ferromagnetic phase where the energy bands are separated into spin-up and spin-down bands. These calculations show a significant difference between the wave vector-dependent susceptibility in the two directions parallel to and perpendicular to the internal magnetic field. The parallel susceptibility which enters into the stability criterion for magnetic ordering has a clear maximum at a wave vector close to the spiral wave vector.

An inelastic neutron scattering study of the microscopic magnetic interactions in the 4f-3d metal alloy $CeCo_5$ was initiated. This material has potential use as a permanent magnet.

The magnetic form factor at small wave vectors can in principle be deduced from the intensity of the spin wave scattering. This method was investigated by measurements on Fe. The results were encouraging, but more experiments are necessary before definite conclusions can be drawn.

Neutron diffraction on $MnCr_2S$ with Se substituting for some of the S showed that the known large increase of the spontaneous magnetization owing to small amounts of Se is not caused by an increase of the canting of the manganese moment.

Measurements of the spin wave renormalization in magnetite showed that spin waves with large wave vectors exist above the curie temperature.

The spin wave renormalization in Heisenberg ferro- and anti-ferromagnets with single-ion anisotropy was derived theoretically, and the theory was applied to the almost 2-dimensional anti-ferromagnets $NiCl_2$ and $CrCl_2$.

The experiments on the lattice dynamics of solid H_2 and D_2 were completed. The phonon energies were found to be very similar in the two solids. The energies agree well with theory if quantum effects are explicitly taken into account. The only pronounced qualitative manifestation of quantum effects was, however, an anomalous variation of the scattered intensity with the scattering vector. The impurity modes in the single-crystal alloys H_2 + 10% D_2 and H_2 + 6% D_2 were investigated. In these substitutional defect systems the change of the force constants - in addition to the mass change - is expected to be very important.

Phonons in crystalline $SrCl_2$ and S_8 were studied by coherent neutron scattering. In S_8 the aim was to measure the intermolecular forces and to compare them with model calculations based on a single, very simple interaction potential between atoms in adjacent molecules.

The hydrogen bonding in deuterated pyrazene and the interaction forces in deuteropolythene were studied by coherent inelastic neutron scattering. Preliminary experiments on incoherent neutron scattering from the liquid crystal ammonium perfluorooctanoate indicate little difference between the diffusion in the plane of the water layers and the diffusion perpendicular to that plane.

The neutron diffraction investigation of amorphous ice was continued, and preliminary results on the structure factor and the radial distribution function were obtained.

Insight in the physics of liquids can be gained from experiments on inelastic neutron scattering. Such measurements on the quantum liquid H_2 were started. The special neutron scattering properties of this liquid allow us to separate coherent from incoherent neutron scattering. Well-defined collective excitations were observed in the coherent scattering law.

Various new experimental methods and techniques were investigated. The application of neutron diffraction to texture studies was tested. Neutron diffraction by moving crystals was tried out as an analysing system and as a neutron-slowing-down method. Equipment for measurements at high pressure was developed as were techniques for producing single crystals of the rare earth metals and alloys.

The plasma physics section works in two fields: basic plasma properties (utilizing a Q-machine) and technology of interest for future fusion reactors (utilizing a puffatron and a magnetically driven shock tube).

The puffatron produces a rotating hot plasma in an $\bar{E} \times \bar{B}$ configuration between two coaxial cylindrical electrodes. In the shock tube a strong shock moving at a constant speed is produced electromagnetically through the interaction between a constant driving current and its self-magnetic field.

In collaboration with Culham (UKAEA, England), studies of the interaction between the plasma and solids injected into the plasma were pursued with a possible refuelling scheme for future fusion reactors in mind. A launcher of solid hydrogen pellets is operating on the puffatron machine; experiments showed that the mass loss of the pellets injected into the plasma is one order of magnitude higher than expected theoretically.

The interaction with the plasma is very complex, depending on effects from different charged particles of different energies. A further experiment is being designed which will allow the bombardment of a solid hydrogen target with well-defined particles in order to get the needed information on basic elemental processes in the plasma - solid interaction. In order to evaluate the performance of the shock tube in connection with possible plasma-solid interaction studies, the electron density, the temperature, and the test time in the shock were measured.

The Q-machine produces a cold dc-plasma (2000 K) from Cs ionized by impact on a hot Ta-plate. The plasma is confined by a constant, homogeneous magnetic field. The propagation of perturbations of the plasma was studied. It was shown experimentally and theoretically that collective interactions are significant only if the electron temperature is a good deal higher than the ion temperature. The Vlasov equation for the ion density was solved without the usual "first pole approximation" and it was shown that this approximation often gives incorrect results.

The nuclear physics section works on problems related to fission. An in-beam experiment for measuring coincidences between fission fragments, conversion electrons, and X-rays at the DR 3 is being built.

The meteorology section is primarily engaged in studies of the planetary boundary layer. Special subjects of interest are: Measuring and analysing techniques, turbulence-spectra and fluxes over land and sea (the air - sea interaction), and climatology.

At Risø a 120-m tower is available for experimental work. Also meteorological parameters such as wind speeds and directions, temperatures, humidity, pressure, and precipitation are measured routinely in the tower at different heights. As a result of these measurements data records are available containing 15 years of hourly readings of these parameters. These records are used extensively by us as well as by others for research purposes.

For field experiments the section has at its disposal a 50-m mobile tower and a data sampling system installed in a van. The sampling system consists essentially of an automatic data sampler capable of sampling 60 channels simultaneously at a rate of 200 times per second.

The data records mentioned above were used in various projects. The characteristics of the vertical profile of the horizontal mean wind velocity were seen to be related to the shape of the terrain which the wind meets on its way to the tower, within the framework of the Monin - Oboukhov theory and also in terms of numerical models. An attempt is being made to construct a numerical model that can treat the connection between local phenomena detected in the tower and meso-scale phenomena. Spectral analyses of the wind and temperature have been completed.

In co-operation with the Geophysical Isotope Laboratory of the University of Copenhagen a statistical analysis of the $0^{18}/0^{16}$ ratio was undertaken on the basis of 800 years of precipitation as stored in the Greenland inland ice. The results have, especially compared with similar results of other workers, revealed interesting information about climatic variations in the northern hemisphere.

In co-operation with oceanographers from the University of Copenhagen and the University of Bergen a tower to be raised in the Kattegat is being constructed. The tower will, among other things, be used for air - sea interaction studies.

This year as earlier, the section undertook a number of tasks of an applied nature. Among them were: Site evaluation and dispersion modelling, development and testing of meteorological instruments, air pollution studies, and evaluation of dynamic effects of wind on building structures.

1. SOLID-STATE PHYSICS (NEUTRON SCATTERING)

Magnetic Structures of Nd in Strong Magnetic Fields

(B. Lebech and B. D. Rainford (Imperial College, London))

Nd has the double hexagonal close-packed structure in which there are two types of sites with cubic and hexagonal environment respectively. Without an applied magnetic field the two types of sites order into periodic antiferromagnetic structures at different temperatures and with different periodicities and moment directions. Upon application of a strong magnetic field in either the b_1- or the b_3-directions of the crystal previous neutron diffraction studies[1-2] have shown that the structures change in a complicated way. Systematic scans through 30 reciprocal lattice points were carried out in applied magnetic fields up to 4.5 teslas. The results are now being analysed.

Magnetic Form Factor of Pr

(B.D. Rainford (Imperial College, London), F. A. Wedgwood (Harwell, England), and B. Lebech)

Pr has the double hexagonal close-packed structure in which there are two types of sites with cubic and hexagonal environment respectively. The measurement of the magnetic form factor of the hexagonal sites performed at the Harwell polarized spectrometer I was extended to .82 $Å^{-1}$ in reciprocal space. Measurements of the magnetic form factor of the cubic sites were initiated. The form factors for the two sites are the same within the experimental accuracy.

Magnetization of Single Crystals of the Light Rare Earth Metals

(K. A. McEwen (H. C. Ørsted Institute), A. R. Mackintosh, G. J. Cock (University of Amsterdam), and L. W. Roeland (University of Amsterdam))

Magnetization of Eu, Sm, Nd, Pr, and PrNd alloys was studied at low temperatures in magnetic fields up to 37 teslas (370 kgaus) in the Amsterdam high-field magnet.

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1) T. Jchansson, B. Lebech, M. Nielsen, H. Bjerrum Møller and A.R. Mackintosh, Phys. Rev. Letters 25 (1970), 524.

2) B. Lebech and B.D. Rainford, Journal de Physique C1 32 (1971), C1-370.

The most striking effects were observed in single-crystal dhcp Pr, where the ionic ground states on both the cubic and hexagonal sites are singlets and the exchange is too weak to induce magnetic ordering at 4.2 K. When a field is applied in the hard [001] direction, as shown in fig. 1, there is an abrupt increase of 1.04 μ_B/atom in the magnetization at 31.5 teslas. This we ascribe to a first-order transition, on the hexagonal sites, from a nonmagnetic to a metamagnetic phase. The transition is sharp to within 0.02 T and shows hysteresis of about 0.2 T.

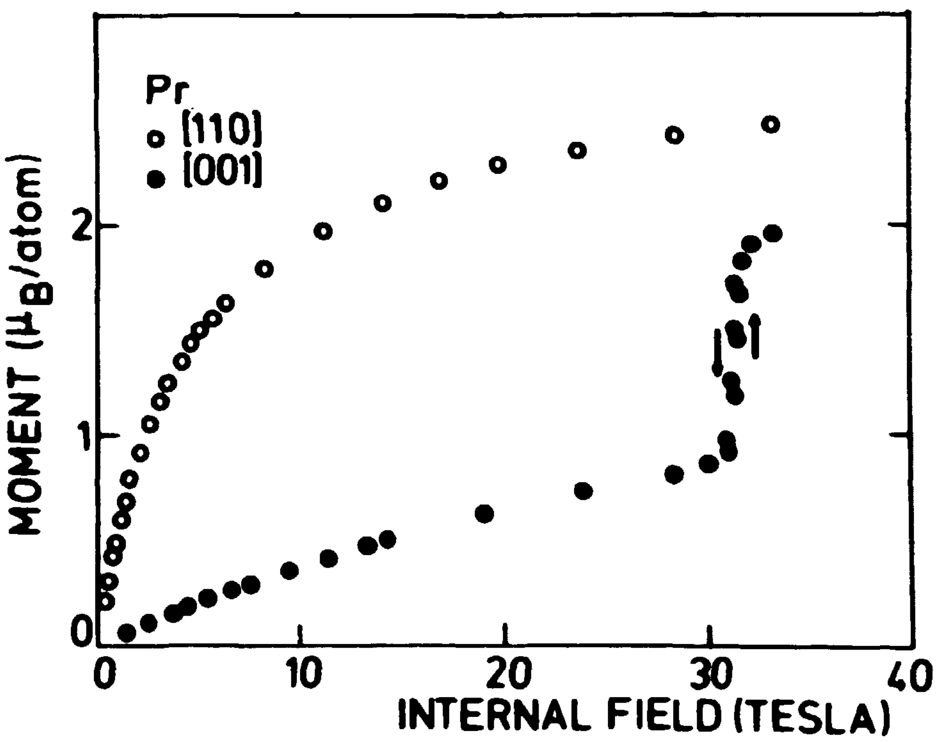

Fig. 1. High field magnetization data for Pr in two directions at 4.2 K. The arrows indicate the observed hysteresis of 0.2 teslas.

It is believed that this transition is due to the crossing of the $|m_J\rangle = |0\rangle$ ground state by the $\sqrt{1/2}\,(|+3\rangle - |-3\rangle)$ level, which mixes with the $\sqrt{1/2}\,(|+3\rangle + |-3\rangle)$ level and drops rapidly in energy on the application of an axial field. From neutron scattering results and the details of magnetization, we hope to deduce the low-lying crystal field levels on the cubic and hexagonal sites.

Exciton Dispersion Relations in Rare Earth Compounds with a Strong Crystalline Field

(Per Bak)

For most rare earth compounds the crystal field is comparable to or even greater than the exchange interaction.

Therefore it is not possible to describe the magnetic excitations as ordinary spin waves where the crystal field perturbs the exchange energy, thus giving rise to anisotropy. Instead it is necessary to consider the crystal field and the exchange field on an equal footing.

The exciton dispersion relations and various thermodynamical quantities for such a multilevel system were derived both in the ordered and in the paramagnetic phase by two different methods.

(1) A double-time Green function technique with a random phase approximation for the decoupling of the equations of motion in a generalized Pauli representation.

(2) A standard field-theoretical method with a boson and a fermion representation. The calculations in the exact fermion representation were carried out for a singlet - singlet system.

Magnetic Properties of Neodymium and Praseodymium Monopnictides

(P. Bak and P.-A. Lindgård)

A molecular field theory for magnetic systems of arbitrary symmetry in which the crystal field is stronger than or comparable to the exchange interaction was developed. It was applied in interpreting magnetic data on various rare earth pnictides[1]. From the complete theoretical expressions for the susceptibility we deduced a set of exchange parameters. As may be seen in the table our exchange parameters differ significantly from those derived from expressions valid at infinite temperatures or for exchange interaction only. Thus we conclude that it is necessary to analyse magnetic data in the rare earth pnictides on the basis of a theory which properly includes the crystal field.

---

1) P. Schobinger-Papamantellos, P. Fischer, O. Vogt, and E. Kaldis, J. Phys. C (1973) (to be published).

Comparison between exchange constants for Nd-pnictides. J_1 and J_2 are nearest and next-nearest neighbour exchange interaction in degrees Kelvin

	OUR	1)	OUR	1)
IN	$12J_1+6J_2$	$12J_1+6J_2$	$6J_2-4J_1$	$6J_2-4J_1$
NdP	.88	.55	.96	.70
NdSb	.10	-.18	1.11	.94
NdAs	.55	.18	1.03	.72

Crystal Field Splittings in the Rare Earth Compounds: $R_xY_{1-x}Al_2$ (R = Pr, Er, Tm) and CeS, CeP, CeAs

(J. K. Kjems, H. Heer and A. Furrer (EIR Würenlingen), and H.G. Purwins (University of Geneva))

The effort to map out the crystal field splittings in metallic and semimetallic rare earth compounds was continued in collaboration with visitors from EIR, Würenlingen. Measurements with the new MARX-spectrometer were performed on compounds of Lave's phase of the type $R_xY_{1-x}Al_2$ (R = Pr, Er, Tm). The polycrystalline materials were diluted with yttrium in order to reduce the line widths due to exchange interactions. The crystal field parameters derived by least-squares fitting agree qualitatively with estimates based on nearest-neighbour point charge models, and they agree quantitatively with susceptibility data.

Well-resolved spectra were obtained from a series of Ce-compounds (CeS, CeP, CeAs) with only two levels, a doublet and a quartet. The transitions were studied as a function of temperature in order to obtain information on line broadening mechanisms.

Crystal Field Splittings in $PrFeO_3$ and Pr_6O_{11}

(K. Henning (Dubna, USSR) and E. Warming)

In $PrFeO_3$ the Pr-ion is a Pr^{4+} ion if it is situated on octahedral sites, and its electronic configuration will be analogous to that of the Ce^{3+} in CeSb. Therefore one expects the ground state to be an $F_{5/2}$ state which is split into a doublet and a quadruplet. We estimate that the inner molecular magnetic field induced by the Fe-ions is not strong enough to split the Pr^{4+} ground state further.

We studied the levels at 4 K by inelastic neutron scattering. At this temperature only the lowest level is populated and therefore only transitions from the ground state to higher levels are observed in a neutron energy loss experiment. We determined one transition energy for both compounds. For $PrFeO_3$ we see indications of more transitions.

Anisotropic Exchange Interaction between the Magnetic Ions in Tb

(J. Jensen, J. Gylden Houman, and P. Touborg (DTH, Copenhagen))

The measurements of the magnetic anisotropy of Tb were continued with studies of the magnetic field dependence of the energies of spin waves propagating in the c-direction at three different temperatures (4.2, 53, and 134 K). A magnetic field of up to 10 teslas was applied both in the easy and the hard direction.

The energies of the elementary excitations of an anisotropic Bose system are described by two parameters A(q) and B(q)[1)] so that

$$E(q) = [\,(A(q) + B(q))\,(A(q) - B(q))\,]^{1/2},$$

where q is the wave vector. The application of a magnetic field increases the energy of the spin waves in a way that makes a separation of the two parameters possible.

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1) H. Bjerrum Møller, J. Gylden Houmann, J. Jensen, and A. R. Mackintosh, Neutron Inelastic Scattering 1972. Proceedings of a Symposium held in Grenoble, March 1972 (IAEA, Vienna, 1972) 603.

The crystal field contributions to the spin wave energies are independent of q, whereas the exchange coupling between moments on different ions is responsible for the q-dependence of the energies. An anisotropic exchange interaction will then be reflected in a q-dependence of the anisotropy parameter B(q).

The interpretation of the experimental results is impeded (1) by an ambiguity in the sign of B(q), (2) by the field dependence of the magnetization, and (3) by the magnon - phonon interaction.

(1) The ambiguity in the sign of B(q), which has led to difficulties in the interpretation for q greater than 0.45 $\mathring{A}^{-1}$, has now been eliminated as a result of studies of the q-dependence of the cross section of the magnons. As shown by P. A. Lindgård et al.[1)] the magnon cross section for neutrons depends on the anisotropy of the spin interaction. This analysis led to an interpretation of the measurements which differs from what has previously been published[2)].

(2) The anormal temperature dependence of the field dependence of the spin wave energies is explained by the increase of the relative magnetization, σ, when a field is applied (the change of σ is negligible at zero temperature). Because of the σ-dependence of the crystal field and exchange parameters, this introduces corrections which at 134 K amount to about 25%.

(3) The observed coupling between acoustic magnons and optical phonons propagating along the c-axis perturbs the field dependence of the magnon energies very strongly. S.H. Liu[3)] has proposed a magnon - phonon interaction involving an intermediate state in which an electron-hole pair is excited virtually by the phonon and subsequently recombines into a magnon. According to this theory the observed interaction becomes possible when the spin-orbit coupling is taken into account. Although the energy difference between long-wavelength acoustic magnons and optical phonons is large, the coupling between these modes is not necessarily negligible, because both the acoustic magnon - electron and the electron - optical phonon interaction amplitudes have maxima at zero wave vector. This means that all magnons, with the exception of long-wavelength optical magnons, are perturbed significantly by the transverse phonons.

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1) P.-A. Lindgård, A. Kowalska, and P. Laut, J. Phys. Chem. Solids 28, 1357 (1967).

2) H. Bjerrum Møller, J. Gylden Houmann, J. Jensen, and A.R. Mackintosh, Neutron Inelastic Scattering 1972. Proceedings of a Symposium held in Grenoble, March 1972 (IAEA, Vienna, 1972) 603.

3) S.H. Liu, Phys. Rev. Letters 29, 793 (1972).

The analysis of the experimental results is not yet finished. However, provisional results for the two exchange parameters are shown in fig. 2 (the magnetization is along an easy direction). The figure also illustrates the strong influence of the magnon - phonon interaction. A proper account of the magnon - phonon interaction will possibly enhance the crystal field anisotropy (deduced at zero wave vector) and hereby reduce the exchange anisotropy shown in fig. 2.

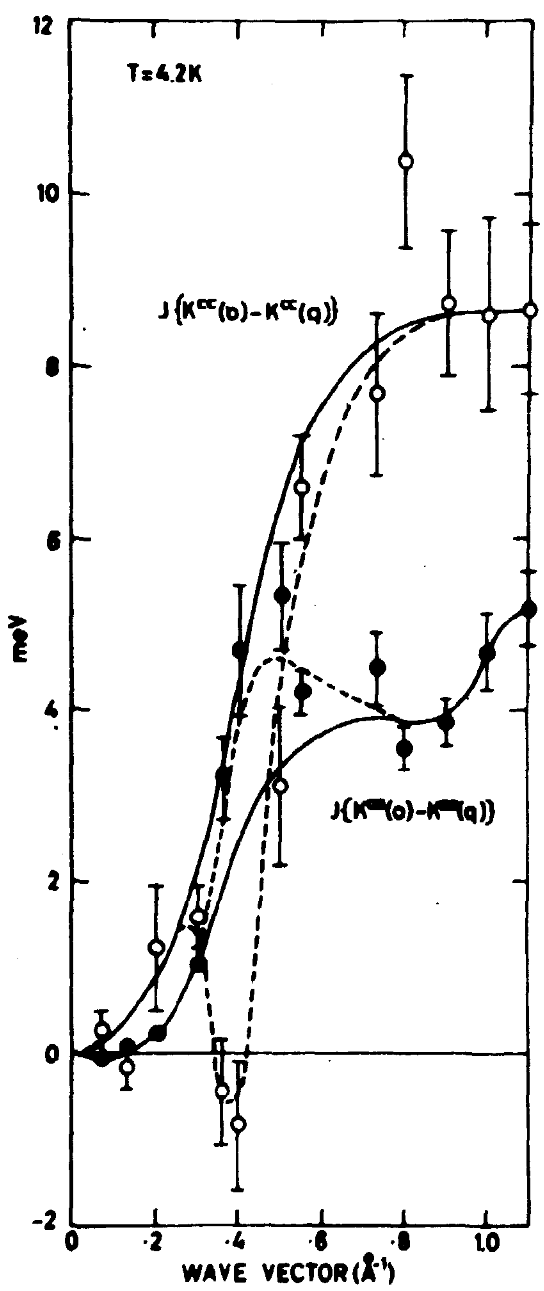

Fig. 2. The Fourier transforms of the effective two-ion coupling between moments for the c-direction of Tb. The symbols connected by the dashed lines are the results when the magnon - phonon interaction is neglected, whereas the solid lines show the provisional results when the interaction is introduced.

Calculation of the Conduction-Electron Susceptibility of Rare Earth Metals in the Magnetically Ordered Phase and Considerations on the Exchange Interaction

(Per-Anker Lindgård)

In the ferromagnetic phase the conduction electron energy bands are separated into spin-up and spin-down bands. The splitting is of the order of 0.02 ryd and is not negligible compared with the width of the bands near the Fermi surface. This splitting gives rise to a difference between the wavevector-dependent susceptibilities, $\chi_q^{\parallel}$ and $\chi_q^{\perp}$, in the directions parallel to and perpendicular to the internal magnetic field. A first calculation for Tb and Dy was based on a "root-sampling" sum program developed by S. Liu et al.[1] and a rigid band splitting. In a crude model the matrix element between a conduction electron and a 4f-electron can be approximated by the conduction electron formfactor. Then the exchange interaction $J_q^{\perp}$ entering into the spin wave dispersion relation is simply given by the formfactor multiplied by $\chi_q^{\perp}$. By comparing a measured $J_q^{\perp}$ and the calculated $\chi_q^{\perp}$ we can thus deduce the conduction electron formfactor. This formfactor only contributes to the total formfactor at small wavevectors. It can in principle be measured directly by inelastic neutron scattering. Using the deduced formfactor and $\chi_q^{\parallel}$ we can therefore find the theoretical $J_q^{\parallel}$ which enters into the stability criterion for the magnetic phase. For both Tb and Dy we find that $J_q^{\parallel}$ shows a clear maximum at a wavevector very close to the spiral vector Q although $J_q^{\perp}$ has no clear maximum.

The band splitting thus enhances the tendency to form a spiral phase. The calculation of the effect of band splitting in the spiral phase shows even further stabilization. The conclusion of this preliminary study is therefore that the back-coupling effects of the localized moments on the conduction electrons give rise to a significant and temperature-dependent variation of the effective interaction between the localized moments. A more complete study has therefore been undertaken in an effort to treat the matrix element in more detail and a program has been written to improve the q-summation by the Gilat - Raubenheimer method.

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1) S. Liu, R.P. Gupta, and S.K. Sinha, Phys. Rev. B, 4, 1100 (1971).

Magnon - Magnon Interactions in the Heavy Rare Earth Metals

(P.-A. Lindgård and O. Danielsen)

The magnon renormalization in a ferromagnet with hcp structure was calculated, using the Hartree - Foch approximation.

The isotropic exchange, single-ion anisotropy terms, and magneto elastic terms relevant for the heavy rare earth metals were included in the Hamiltonian. The temperature dependence of the energy gap, of the magnetization, and of the macroscopic anisotropy parameters were calculated. The temperature variation of the macroscopic anisotropy constants deviates from the simple $l(l+1)/2$ law when the effects of zero point motion and magneto elastic terms are included.

Spin Waves in the Permanent Magnet $CeCo_5$

(L. Holmes and J. Als-Nielsen)

In recent years alloys of rare earth metals and 3d transition metals have been studied intensively because of their potential usefulness as permanent magnets. Nevertheless, the microscopic interaction between the atomic magnetic moments has not been revealed at all since none of these alloys have been studied by inelastic neutron scattering. We attempted such a study, but although spin wave scattering was observed, it was not possible to obtain any detailed picture because the sample mosaic spread was very wide ($\sim 10^o$). There is no doubt about the feasibility of such an experiment when good single crystals become available.

Magnetic Form Factor in Fe at Small Wave Vectors by Intensity Study of Neutron Spin Wave Scattering

(J. Als-Nielsen and G. Shirane (Brookhaven, U.S.A.))

The magnetic formfactor, which is the Fourier transform of the spatial distribution of the magnetic moment density, is in ferromagnets conventionally measured by Bragg scattering of polarized neutrons. With this method, therefore, the smallest wavevector at which the formfactor is being determined is the shortest reciprocal lattice vector with an allowed Bragg reflection. In addition, the bulk saturation magnetization determines the formfactor at zero wavevector. In iron, the formfactor at wavevectors $q \geq \tau_{110} = 3.06$ Å^{-1} is in close agreement with calculations based upon the unpaired 3d electron atomic orbitals only. On the other hand the formfactor at $q = 0$ is about 10% lower than an extrapolation of the calculated 3d formfactor. This has been interpreted as being due to a negatively polarized sea of 4s conduction electrons in the metal.

The formfactor in the formula for the neutron scattering cross sections is, of course, the total formfactor, i.e. the sum of 3d and 4s in the above case.

We have attempted to gain information about this formfactor in the range $0.03\ \text{Å}^{-1} \leq q \leq .12\ \text{Å}^{-1}$ from the intensity of the spin wave scattering around the forward direction, the integrated intensity in an energy scan at fixed modulus q being proportional to the formfactor $|f(q)|^2$. The dominant contribution to the q-dependence of this integrated intensity comes from the susceptibility $\chi(q) \sim q^{-2}$, and it is the formfactor variation on top of that which we attempt to extract from the data. Furthermore, at a certain wavevector transfer q, only a limited region of energy transfers are kinematically possible, and this energy range is particularly limited in inelastic scattering around the forward direction. In order to get an appreciable part of the spin wave spectrum at a certain q within the accessible energy range, it was necessary to lower the spin wave energies by heating the sample to a temperature about 3% below the curie temperature. Finally the resolution ellipse (i.e. the shape in (q, ω) space of the neutron probe) varies considerably in size and orientation in scattering around the forward direction, and a detailed knowledge of this effect is necessary if reliable information about the formfactor from the data is to be obtained.

Our preliminary results on this basic problem in the ferromagnetism of 3d metals are encouraging, but more experiments and analyses are required before definite statements about the formfactor at small wavevectors in iron can be made.

Magnetic Structure of Se-substituted $MnCr_2S_4$ Spinels

(L.M. Holmes and B. Lebech)

The substitution of Se for S in $MnCr_2S_4$ produces dramatic changes in the magnetic ordering (e.g., the spontaneous magnetization M_0 at low temperatures increases 50% while the curie temperature T_0 decreases 3%, when as little as 2.5% of the S is replaced by Se[1)]). In order to understand these effects a neutron-diffraction study at low temperatures has been

[1)] M. Robbins et al., Conf. on Magnetism and Magnetic Materials, Denver, 1972.

initiated in the substituted cubic materials $MnCr_2S_{4-x}Se_x$, with $0 \leq x \leq 1$. The unsubstituted $MnCr_2S_4$ is ferrimagnetic below T_c = 74 K and undergoes a second magnetic transition at $T' \approx 5$ K. At $T < T'$ the measured M_o is greater than the 1 μ_B expected from the difference in Cr^{3+} $(2 \times 3\mu_B)$ and Mn^{2+} $(5\mu_B)$ moments. This is known[1] to be due to canting of the Mn^{2+} moments with respect to the Cr^{3+} moments - the Yafet - Kittel model. The canting gives rise to a finite intensity in the (002) reflection (see fig. 3), which is forbidden in a collinear structure. The increase in M_o on adding Se might be due to increased canting, but this possibility was not supported by the observed diffraction pattern for the Se-containing samples, in which the (002) reflection was entirely absent at T = 2 K. A more detailed study of the magnetic structure in the series of compounds is therefore being carried out.

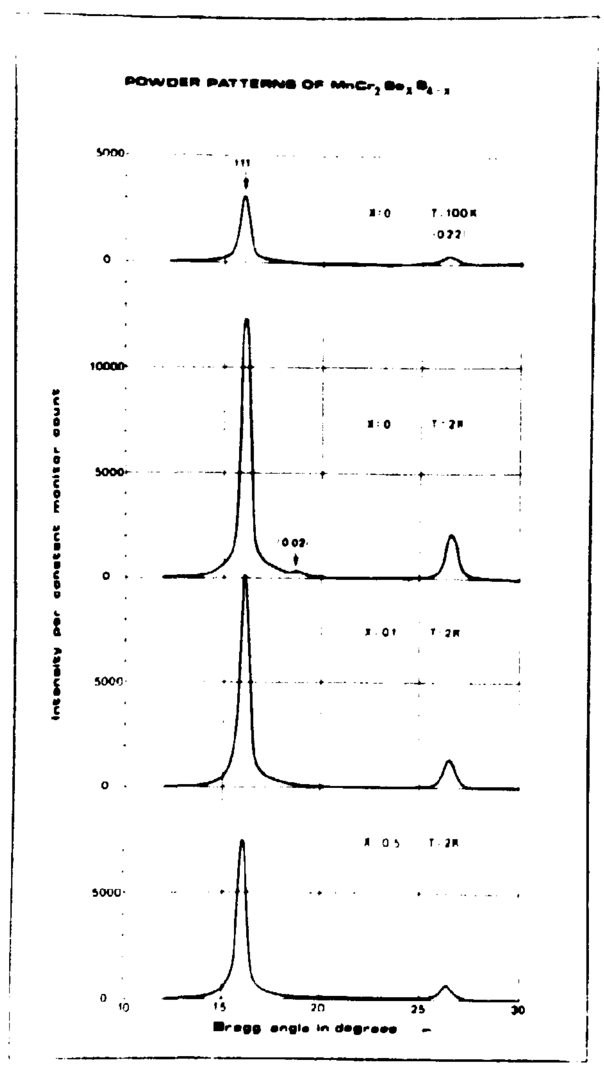

Fig. 3. Neutron diffraction patterns of Se-substituted $MnCr_2S_4$ spinels at a neutron wavelength of 1.65 Å. A smoothed background correction has been applied to the data. The increase in intensity between the 100 K and 2 K patterns is due to magnetic ordering. Note the small (002) reflections which appear only for the unsubstituted $MnCr_2S_4$ ($x = 0$), and which are due to canting of the Mn sublattice moments.

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[1] R. Plumier and M. Sougi, C.R. Acad, Sc. Paris, 268 B, 1549 - 1552 (1969).

Renormalization of Magnons in Magnetite

(M. R. Evans (Cambridge, England) and E. Warming)

The energies of the acoustic magnons of small wavevectors renormalize to zero at the critical temperature T_c = 835 K as shown by Collins and Saunderson[1]. We have looked for similar effects for magnons of larger wavevectors, using triple-axis spectrometers at Harwell and at Risø. The measurements were carried out for wavevectors in the [001] direction.

A renormalization was seen, but in contrast to the magnons measured at small wavevectors the energies are still finite at T_c. The magnons disappear slowly above T_c. It is so far not clear whether this happens because the magnons lose intensity or because of line broadening.

Spin Wave Theory of Ferro- and Antiferromagnets with Planar Anisotropy. Application to the Planar Antiferromagnets $NiCl_2$ and $CrCl_3$

(Per-Anker Lindgård, work performed during a visit to the Bell Laboratories, U. S. A.)

The theory of spin wave renormalization in Heisenberg ferro- and antiferromagnets with single-ion anisotropy was derived using the Born approximation to first order. The sublattice magnetization for the planar antiferromagnets (metamagnets) $NiCl_2$ and $CrCl_3$ was calculated and compared with experiments. With fixed parameters obtained from spin wave measurements in $NiCl_2$ it is possible to obtain an excellent agreement between the experimental $NiCl_2$ sublattice magnetization and the renormalization theory in a temperature range up to more than 50% of T_N. Only one adjustable parameter was used, the interplanar exchange constant. For $CrCl_3$ the renormalized theory agrees with the experimental data and gives essentially the same result as the theory of Narath and Davis[2]. However they used an effective temperature-dependent anisotropy field. It was demonstrated that the sublattice magnetization is extremely sensitive to the value and the temperature variation of the spin wave energy gap at $q = 0$ and thus depends on assumptions about the origin of the anisotropy. In the present theory the renormalization of the full spin wave spectrum is calculated self-consistently.

1) M. F. Collins and D. H. Saunderson, J. Appl. Phys. 41, 1433 (1970).

2) A. Narath and H. L. Davis, Phys. Rev. 137, A163 (1965).

Phonons in Solid H_2 and D_2

(M. Nielsen)

The measurements of phonon energies in the pure solids of H_2 and D_2 have been completed. The crystal growing technique was improved and very large single crystals of pure parahydrogen were grown. Phonon measurements were performed on these crystals along all the high symmetry directions and along some of the zone boundaries of the Brillouin zone of the hcp crystal structure. Also incoherent neutron measurements were done with the big single crystals and the Debye-Waller factor was determined both in the c-direction of the hcp crystal and in the a-direction.

Our main conclusions from the phonon measurements on H_2 and D_2 are the following:

The measured dispersion curves are in rather good agreement with theoretically calculated curves when comparison is made with the self-consistent phonon frequencies. However, in these calculations the short range correlation in the motion of neighbouring particles is taken into account. In such a case the phonon frequencies ought to be deduced by means of the displacement - displacement correlation function. If this is done, the calculated phonon frequencies are larger then the experimental values. The discrepancy amounts to 35% for the longitudinal phonons at the highest energies.

It was found that the experimental dispersion curves can be fitted to third-nearest-neighbour Born von Karman-curves. The parameters of these fits were used to calculate the density of states, the specific heat, and the elastic constants. The Debye temperatures are 114 K for D_2 and 118 K for H_2. The phonon energies are very similar in the two solids, because the increased zero point vibrations in H_2 as compared with D_2 expand the crystal so that the effective-force-constants are substantially softened and this nearly cancels the effect of the mass difference. The Debye temperatures were found to be in agreement with specific heat measurements, but the sound velocities determined by the elastic constants were found to be about 10% higher than recent experimental values.

The large amplitudes of the zero point vibrations in these crystals have been directly observed through the scattering intensities. In solid para H_2 the molecules are in the $J = 0$ rotational state and the cross section for the neutron to scatter a $J = 0$ molecule into the $J = 1$ rotational state is a pure incoherent cross section. By studying the dependence on the scattering angle of the integrated intensity of this rotational transition, which sets in at 14.6 meV, we could measure the Debye-Waller factor directly and with great accuracy. We found that the thermal amplitude for the molecules is the same in the c-direction as in the a-direction. The mean square amplitudes are $\langle u^2 \rangle = 0.48 \pm .03\ \text{Å}^2$.

Also the coherent scattering intensities in H_2 and D_2 were found to be very different from the scattering intensities in a classical harmonic solid. The integrated intensity of the measured neutron groups was corrected for the variation of the harmonic one-phonon cross section. The thus reduced intensity has a strong anomalous variation as a function of the scattering vector $\bar{\kappa}$. This is shown in fig. 4.

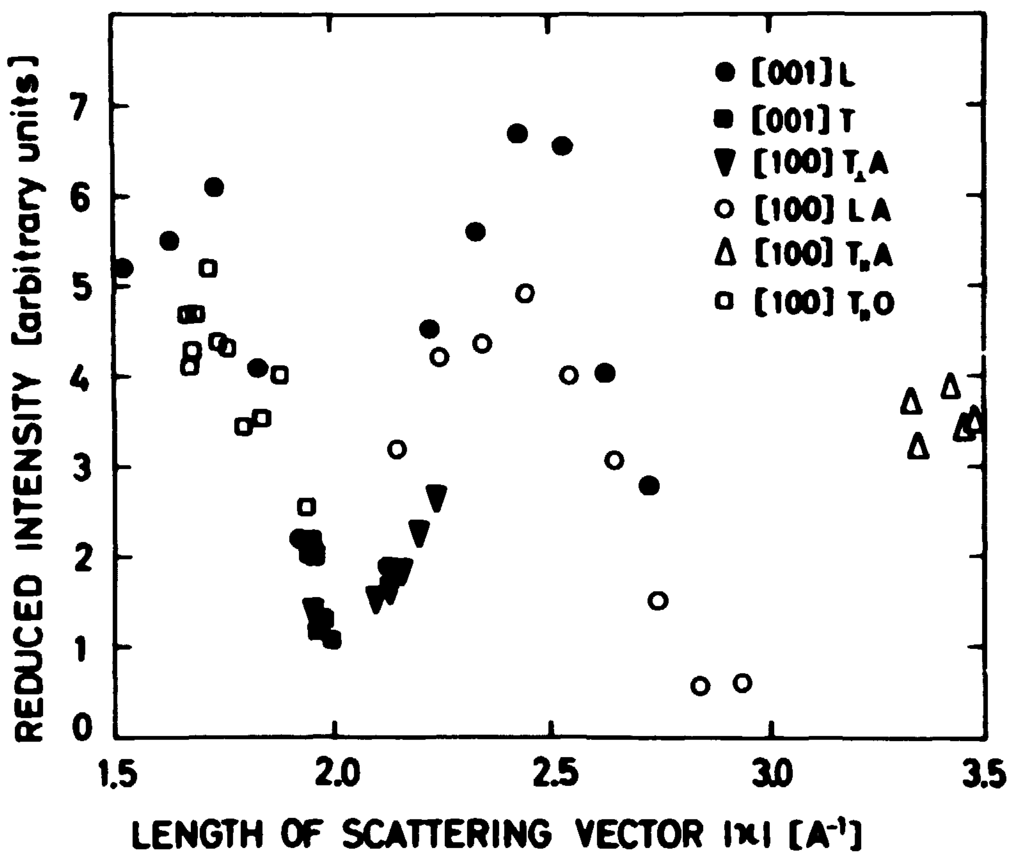

Fig. 4. Reduced one-phonon scattering intensities in solid H_2. The measured intensities were corrected for spectrometer sensitivity and for the variation in the harmonic one-phonon cross section, where the Debye-Waller factor was taken from the incoherent measurements as described in the text.

The natural width of the phonon groups in solid H_2 was also studied. Our first neutron scattering results on solid H_2 showed rather broad neutron groups. However, this was shown to be due to the incoherent scattering from ortho-molecules originating from an imperfect ortho - para conversion prior to condensation. In the final measurements where special precautions were taken in order to ensure complete conversion, the neutron groups were found to have a natural width of 10% of their energy for the highest energies of the longitudinal phonons, whereas the transverse acoustical phonons have a very small natural line width.

Finally we compared the effect on the phonon energy of changing either the pressure, the temperature, or the isotopic mass. This comparison was made for the phonons with wavevector in the c-direction. The parameter deciding the phonon energy shifts is the density of the crystals. It was found that when the density is changed by heating the crystal or by changing the isotopic mass, the phonon energy shifts are larger than when the density is varied by applying external pressure. Further, in all cases the transverse phonon energies are changed more than the longitudinal phonon energies. In these comparisons the phonon energies for solid H_2 have been divided by two to account for the harmonic isotope effect.

Impurity Modes in Hydrogen - Deuterium Alloys

(B. M. Powell and M. Nielsen)

The substitution into a crystal lattice of atoms whose mass differs from that of the host atoms may produce two pronounced effects. If the defect atom is heavier than the host atoms, a resonance appears within the host phonon band; if, on the other band, the defect atom is lighter than the host atoms, a localized mode appears with a frequency greater than the host phonon frequencies. Hydrogen - deuterium alloys are of particular interest in studies of impurity modes because (1) there is a large difference in the coherent scattering lengths of the host and the defect (2) both host and defect form quantum solids, and from measurements of their phonon dispersion curves[1,2] force constant changes are expected to be very important in the defect crystal, and (3) the host lattice has a hexagonal structure rather than the cubic structures considered previously.

These resonance effects were measured in single-crystal alloys with the composition H_2+10%D_2 and H_2+6%D_2. The crystals were oriented with the basal plane as the scattering plane, and observations were made along the [100] and [110] directions. The most striking effect observed was a broad resonance peak in the scattered neutron distributions (fig. 5) in addition to the host phonon peaks. The resonance peak is seen in both alloys and its frequency is approximately that predicted by simple mass defect theory[3]. The observed intensity of the resonance peak relative to

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1) M. Nielsen and H. Bjerrum Møller, Phys. Rev. 63, 4383, 1971.

2) M. Nielsen, Phys. Rev. (to be published January 1973).

3) R. J. Elliott and D. W. Taylor, Phys. Roc. Soc. (London) 296, 161, 1967.

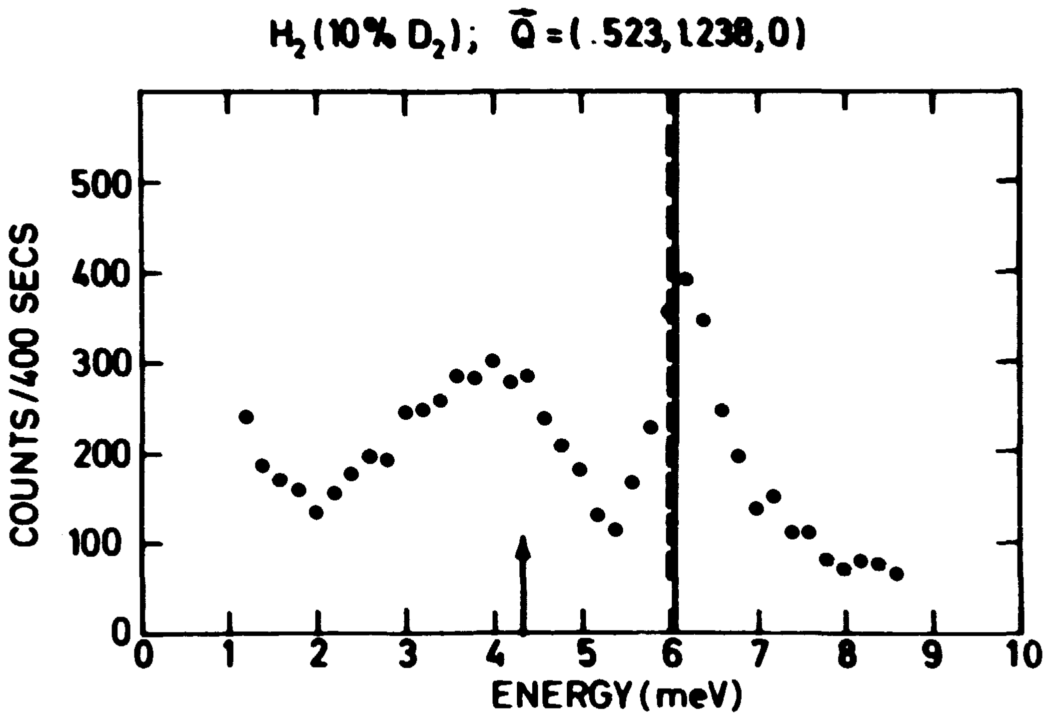

Fig. 5. $H_2(10\% D_2)$. Momentum transfer $Q = (0.523, 1.238, 0)\frac{2}{a\sqrt{3}}$. [110] TA mode. Filled circles are experimental points. The solid vertical line is the energy of the phonon in pure H_2. The dashed vertical line is the energy of the phonon in the defect crystal as predicted by mass defect theory. The vertical arrow is the energy of the resonance mode as predicted by the same theory.

that of an accompanying phonon is generally larger than that predicted theoretically. However, its intensity variation within the zone is in qualitative agreement with calculation. Phonons of the host crystal with frequencies below the resonance frequency are generally shifted to lower frequencies in the defect crystal (fig. 6) in agreement with theory. But the magnitude of the shift is smaller than that predicted. Phonons of frequencies above the resonance are either not shifted or shifted to higher frequencies, in disagreement with theory. The measurement were also compared with a self-consistent mass defect theory[1]. However, the predictions of this theory differ only marginally from those of the simple theory. Calculations are in progress to remove the approximation of cubic symmetry in the simple theory to make it more applicable to the present alloy systems.

When 10% H_2 is added to D_2, simple theory predicts that a local mode will appear at 11.2 meV, just above the D_2 phonon band (: 0.1 meV). Measurements were made on a powder sample of D_2+10%H_2 in an effort to observe this local mode. Observations were made at six momentum transfer from 1.3 A^{-1} to 3.5 A^{-1} with energy transfer up to the J = 0 → 1 rotational energy in H_2 (14.5 meV). The local mode was not observed.

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[1] D. W. Taylor, Phys. Rev. 156, 1017, 1967.

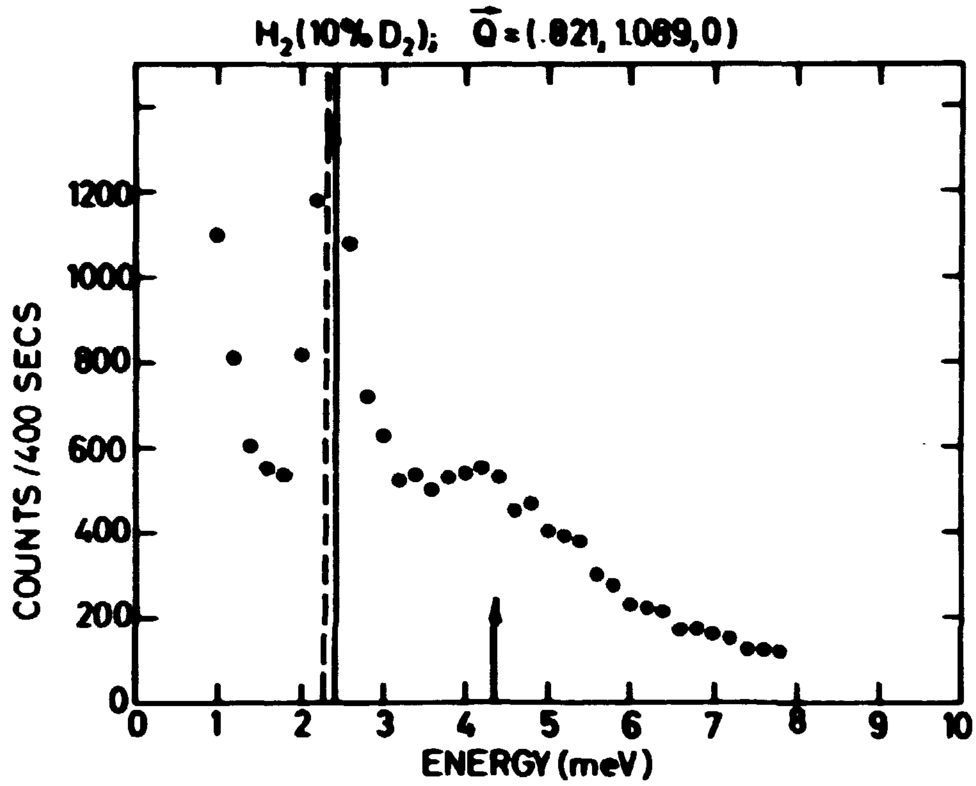

Fig. 6. H_2(10% D_2). Momentum transfer Q = (0.821, 1.089, 0) $\frac{2}{a\sqrt{3}}$, [110] TA mode. The symbols are as described in fig. 5.

Phonon Dispersion Relations of $SrCl_2$

(B. Buras and J.G. Houman)

In view of the growing interest in the lattice dynamics of fluorite structures and following the suggestion of W. Hayes (Clarendon Laboratory, Oxford) measurements of phonon dispersion relations in strontium chloride single crystals were started. A triple-axis spectrometer and the neutron inelastic scattering method are used. Until now the acoustical bronches in the high symmetry directions Γx and Γk have been measured.

Phonons in Crystalline S_8

(J.K. Kjems, R. Rinaldi, and G.S. Pawley (University of Edinburgh))

The intermolecular forces in S_8 crystals were studied by measurements of the low-frequency phonons which correspond to motions of the molecules as rigid units. The orthorhombic crystal structure contains four molecules per unit cell which gives rise to a total of 24 branches neglecting the internal degrees of freedom of the molecules. At symmetry points in the reciprocal lattice this number is reduced, and the inelastic neutron structure factor selects only a few to be observed in a given scan. The main problem is that of assignment of the observed excitations. In this case this assignment is only possible because a relatively reliable model calculation is at hand. The ultimate aim of the experiment is to test this particular model which is based on a single very simple interaction potential between atoms in adjacent molecules. A preliminary analysis revealed a good correspondence between calculated and observed structure factors and a fair agreement between the corresponding frequencies.

Hydrogen Bonding and Phonons in Pyrazine

(P. A. Reynolds)

A single, twined crystal of deuterated pyrazine ($C_4N_2D_4$) was grown from the melt. The crystal structure is sufficiently simple (Pnam with 2 rigid molecules in the unit cell) for the dynamical behaviour to be dominated by D..... D and C-D..... N interactions, the latter being hydrogen bonding. With coherent neutron inelastic scattering a complete set of adiabatic elastic constants (9) was obtained at room temperature. 21 of the 27 lattice modes at symmetry points in the twin plane ($\xi\eta\xi$) were observed together with a set of dispersion curves in the ($0\eta0$) direction. Eigenvectors were assigned to these modes by comparison of observed and calculated inelastic scattering intensities. The observed eigenvalues were fitted to a simple dynamical model, taking into account the eigenvector assignments to remove ambiguity. This model employs an atom-atom potential together with an electrostatic interaction between the nitrogen lone-pair electrons and the C-D dipole to simulate the hydrogen bonding in the quasiharmonic approximation. All the potential constants are known except the three constants of the C-D..... N bond. Adjustment of these results in a better than 7% ($\omega_{obs} - \omega_{calc}/\omega_{obs}$) fit. This demonstrates that the dynamical behaviour of such a long-range hydrogen bond may be represented accurately by a potential of the form

$$V = \sum_{ij} - \frac{A}{r_{ij}^6} + B \exp(-Cr_{ij})$$

plus an electrostatic interaction.

Corrections to the Atom-Atom Intermolecular Potential in p-$C_6D_4Cl_2$

(P. A. Reynolds)

If we represent the intermolecular potential of p-$C_6D_4Cl_2$ by

$$V = \sum_{ij} - \frac{A}{r_{ij}^6} + B\exp(-Cr_{ij})$$

where $\sum_{ij}$ is a sum over all pairs of atoms in the two molecules and A, B, C are constants depending only on the chemical nature of the atoms, then this is a good representation of the cynamical and structural behaviour of the chlorobenzenes. This potential, which implies isotropic molecular polarizability and no molecular electric moments, does not represent the sublimation energies well. The dominant electrostatic forces may be introduced by adding the C-Cl-bond dipole moments observed experimentally in chlorobenzenes. The intermolecular London dispersion energy may be written more accurately by use of the refractive index and of ultra-violet spectral data to fix a single constant in the transition monopole approximation.

These corrections improve the fit of the sublimation energy while the dynamics and the structure are very little affected, thus showing that the initial neglect of these forces is justified, and that errors in the dynamical fit arise mainly from the repulsive part of the potential.

Lattice Dynamics of Deuteropolythene

(J. F. Twisleton (Oxford University, England) and P. A. Reynolds)

In order to elucidate the interchain forces in deuteropolythene coherent inelastic neutron scattering measurements were performed along the chain direction and in the perpendicular plane. Both the basal plane and the chain directions were partially oriented with mosaic spreads of 17^o and 7^o respectively. The three zone-centre modes observed in this partially oriented polycrystal are reproduced quite well by a simple atom-atom potential for the interchain forces, on the assumption of the chains being rigid.

Quasi-elastic Scattering in Water Layers

(J. W. White and J. B. Hayter (Oxford University), and P. A. Reynolds)

Ammonium perfluorooctanoate is a liquid crystal containing infinite 2-dimensional layers of water whose thickness may be varied from 9 Å upwards, reproducibly. These layers may be aligned by rolling.

Preliminary high resolution (0.1 meV) MARX spectrometer measurements of the incoherent quasi-elastic broadening indicate little difference in diffusion of water molecules in the plane of the layers and perpendicularly to them, confirming data of lower resolution taken at Harwell in collaboration with A. M. Hecht. Use of higher resolution permits the effect of disturbing near-elastic rotational and other small energy transfer inelastic components to be assessed.

Structure of Amorphous Ice

(J. Wenzel, C. U. Linderstrøm-Lang (Chemistry Department), and S. A. Rice, (University of Chicago))

Neutron diffraction experiments begun last year were continued to determine the structure of amorphous ice, a metastable non-crystalline ice which is prepared by deposition of water vapour onto a surface cooled to below about 100 K[1].

Two-millimeter-thick deposits were prepared on a cadmium substrate plate mounted in a specially designed cryostat, and the scattered intensity for momentum transfers Q from 0.5 $Å^{-1}$ to 7.5 $Å^{-1}$ was measured using 1.27 Å neutrons. This is shown in fig. 7 for a 100 K amorphous ice deposit. As a normalization standard, the scattering from a thin vanadium sheet was also measured.

Because the amount of sample in the scattering volume became smaller as the scattering angle increased (a geometrical effect), it was necessary to normalize the sample intensity with the vanadium standard. This correction was rather uncertain owing to incomplete knowledge of the shape of the amorphous ice deposit. After corrections were made, the structure factor S(Q) was calculated and Fourier-transformed to yield a radial distribution function (RDF).

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1) D. S. Olander and S. A. Rice, Proc. Nat. Acad. Sci. USA, 69, 98 (1972)

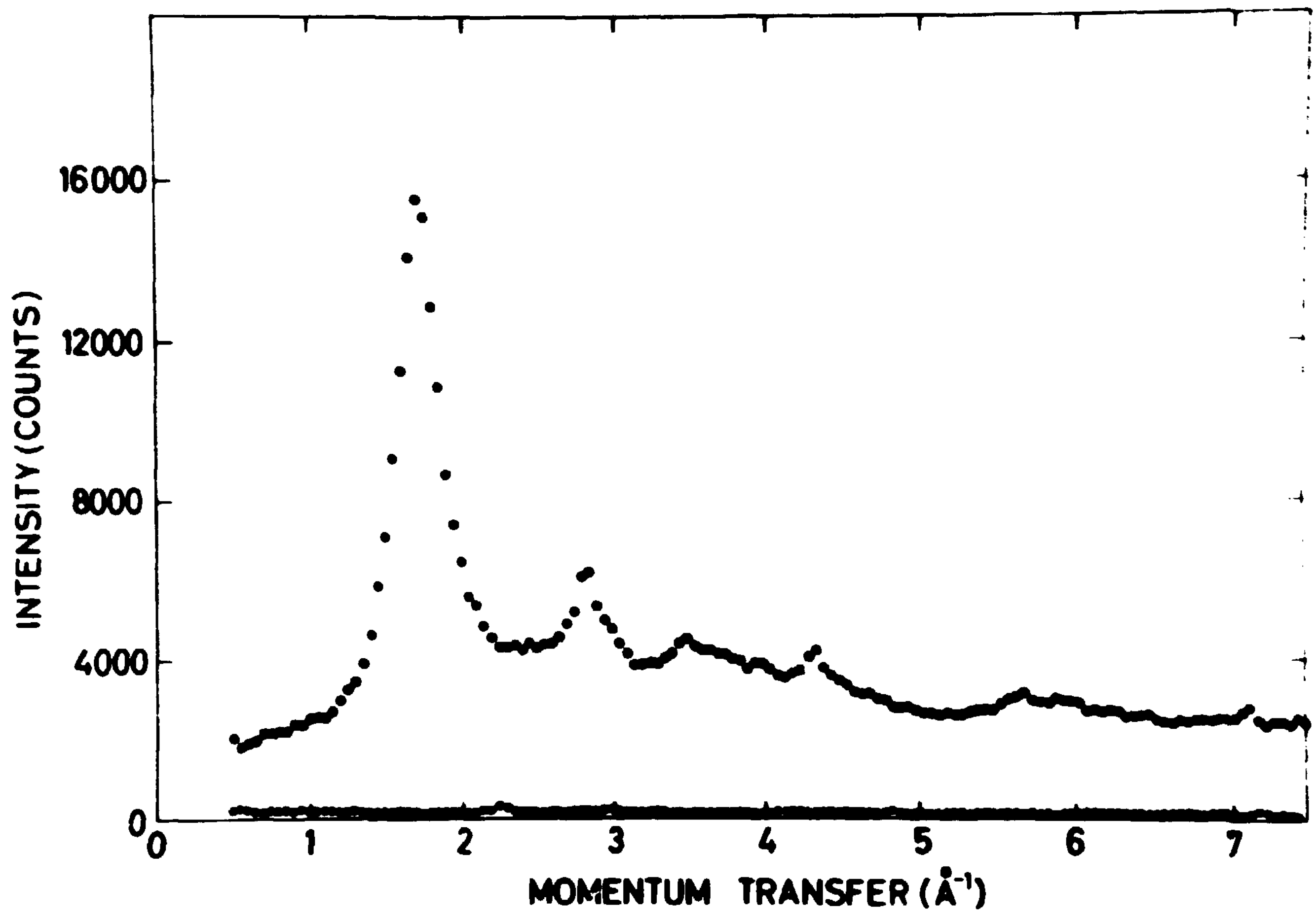


Fig. 7. Measured scattered intensity (top series of points; the background has been subtracted) and the background (lower points) plotted vs. Q, the momentum transfer, for an amorphous D_2O ice deposit made at 100 K. For $Q \geq 3$ Å^{-1} not all of the sample is in the scattering volume and there is a corresponding loss of intensity which has not been corrected for.

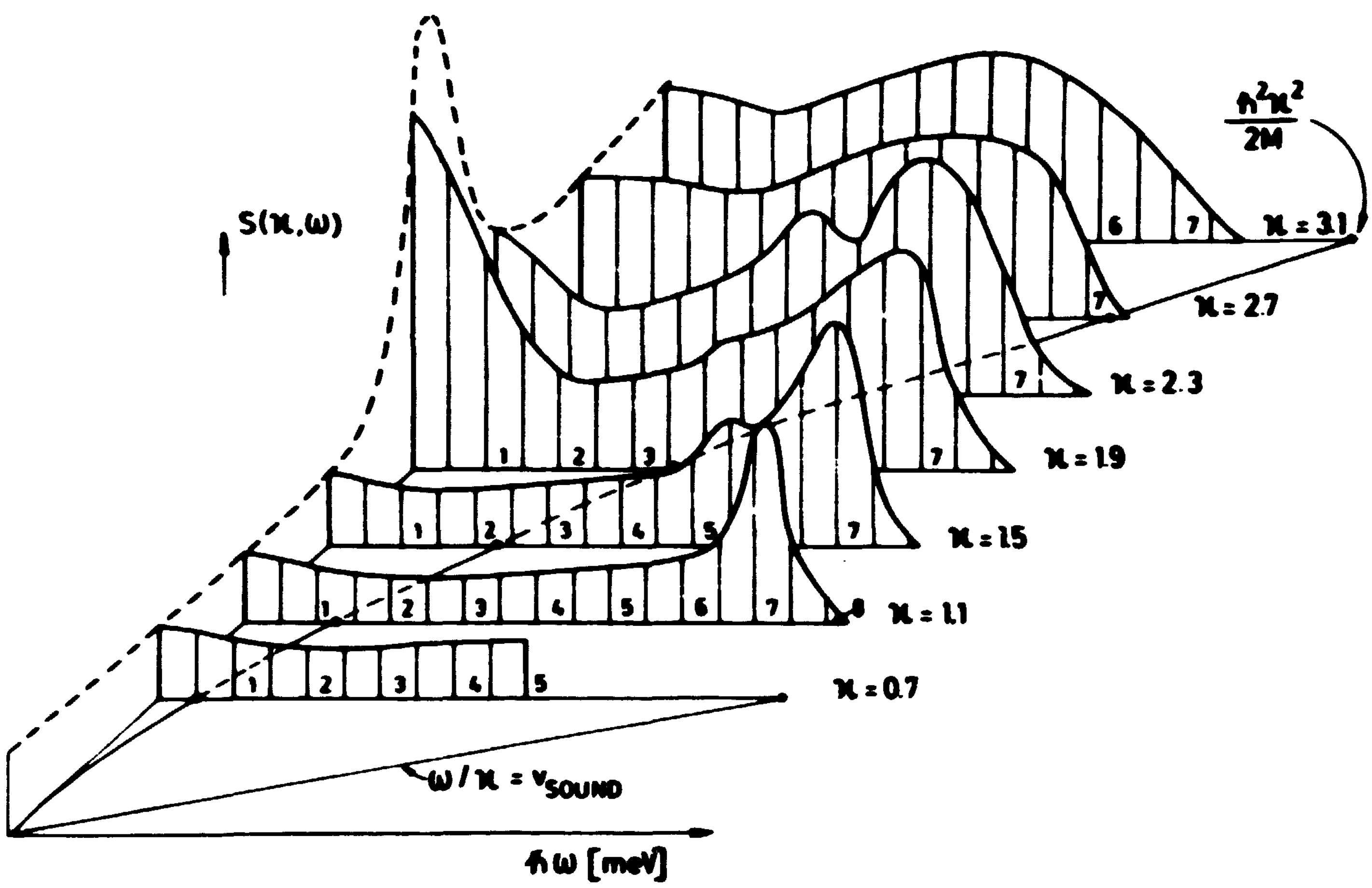
It was found that the computed RDF was quite sensitive to both the method of normalization and extrapolations of S(Q) to Q = 0 and Q = ∞. These difficulties showed the need to measure to both larger and smaller momentum transfer values and to design an experiment to eliminate the geometrical correction. Work along these lines is in progress.

Neutron Scattering in Liquid H_2

(K. Carneiro)

Coherent and incoherent inelastic neutron scattering experiments were made with liquid parahydrogen (rotational quantum number J = 0). These measurements are of special interest for the following two reasons: (1) liquid H_2 is a quantum liquid intermediate between He and Ne. (2) Molecular H_2 has very special neutron scattering properties. In the J = 0 state all scattering at energy transfers below 14.6 meV is completely coherent, whereas neutron scattering at energy transfers above 14.6 meV is incoherent. Since the width of the coherent spectrum is only about 8 meV, a separation of the coherent and incoherent neutron scattering is possible, allowing a determination of the total and self-correlation functions. This is a unique and important property of H_2.

From the coherent scattering the scattering law $S(\kappa, \omega)$ can be obtained (shown in fig. 8). From the form of $S(\kappa, \omega)$ it is seen that well-defined collective excitations exist in this liquid. $S(\kappa,\omega)$ is qualitatively similar to what is observed in liquid ^{4}He, but whereas in ^{4}He only longitudinal excitations are present, transverse modes seem to exist in liquid H_2. This suggests a direct comparison with the one-phonon scattering law of a polycrystal.



SCATTERING LAW FOR LIQUID HYDROGEN

Fig. 8. Scattering law $S(\kappa,\omega)$ for liquid parahydrogen, T = 14.7 K. Complete spectra could not be observed below K = 1.1 $Å^{-1}$ owing to the high velocity of sound. In the base plane the recoil energy curve is shown.

The incoherent measurements yield a diffusion constant, $D = 4.7 \times 10^{-5}$ $cm^2 s^{-1}$ at 14.7 K, consistent with that found by Egelstaff[1]. Also the Debye-Waller factor was deduced. The result corresponds to a mean square displacement $\langle u^2 \rangle = .65$ $Å^2$.

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[1] P. A. Egelstaff, B. C. Haywood, and E. J. Webb, Proc. Phys. Soc. 90, 681 (1967).

Texture Studies by Means of Neutron Diffraction

(T. Leffers (Metallurgy Department), B. Buras, and K. Carneiro)

A preliminary investigation on neutron diffraction methods as a tool to study textures was carried out. Because of the much larger penetration depth neutrons should be superior compared with X-rays in texture studies of coarse grains or not too heavily deformed metals. The method was tested on a copper sample rolled to 40% reduction, and the (111) pole figure obtained is shown in fig. 9. Compared with the pole figure obtained with X-rays the neutron pattern is smoother, which satisfies expectations. The work will be continued with other samples.

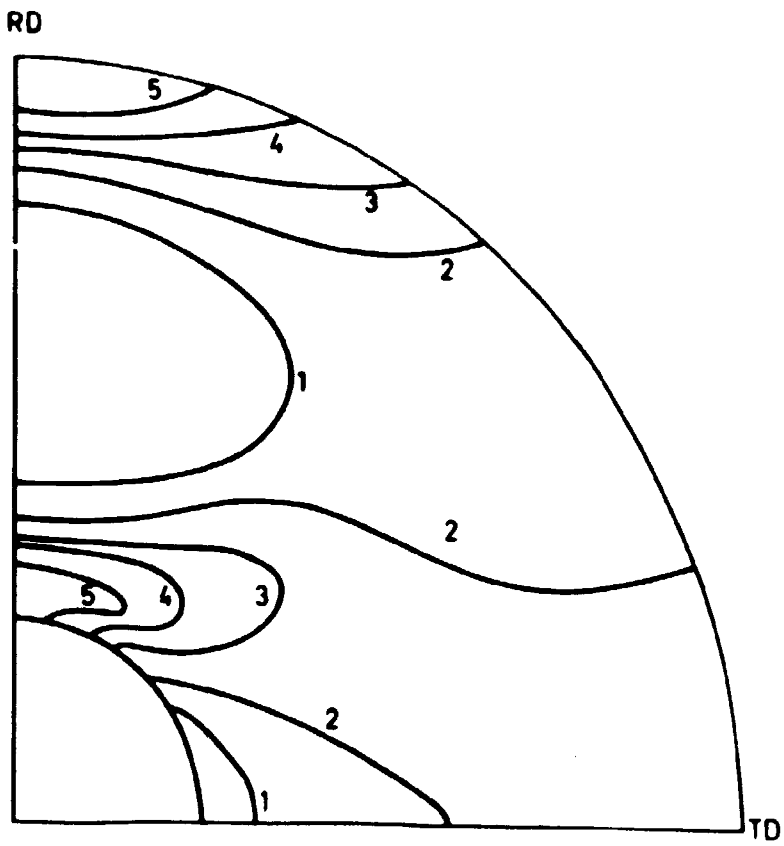

Fig. 9. Pole figure obtained by the neutron diffraction method for the (111) reflection of copper rolled to 40% reduction. Intensities are shown in an arbitrary scale.

Structure Studies under High Pressure

(B. Buras, B. Lebech, and W. Kofoed)

An apparatus for neutron diffraction studies of powdered samples under pressures up to 50 kbars is under construction. The high pressure cell is by necessity designed in such a way that only a few discrete scattering angles (30^{o}, 60^{o}, 90^{o}, and 120^{o}) are possible. This imposes severe limitations on the experiments possible. In an attempt to lift these limitations two fixed scattering angle methods for crystallographic studies were proposed and checked experimentally.

In one method - the analyser scan method (AS) - a polychromatic neutron beam is scattered through a fixed angle by the powdered sample. The wavelength distribution of the scattered neutrons is subsequently analysed by means of a single crystal analyser. In the monochromator scan method (MS) sample and analyser are interchanged. A monochromatic neutron beam of varying neutron wavelength is scattered under a fixed angle by a powdered sample and the intensity of the scattered neutrons is measured as a function of incident neutron wavelength.

Fig. 10 shows diffraction patterns for a silicon powder as obtained by these methods. Both these methods show resolutions and sensitivities comparable to those of the conventional powder method. Thus both methods seem suitable for the study of lattice parameters and of phase changes. The analyser scan method is not very suitable for quantitative structure determination since both the intensity of the incident neutrons and the reflectivity of the analysing crystal varies with neutron wavelength. The monochromatic scan method, on the other hand, may be used for quantitative structure determination since the intensity of the incident neutron beam can be monitored and the integrated intensities of the Bragg peaks can be normalized.

Neutron Scattering from Samples under Moderately High Pressure

(K. Carneiro, W. Kofoed)

A chamber to be used for neutron scattering on samples at liquid-helium temperature and pressure up till 6 kbars is being constructed. A Hg piston keeps the oil of the hydraulic pressurizing pump away from the sample.

The sample container, so far only made for 2 kbars, is designed so that all scattering angles are accessible. The first experiment will be on liquid hydrogen.

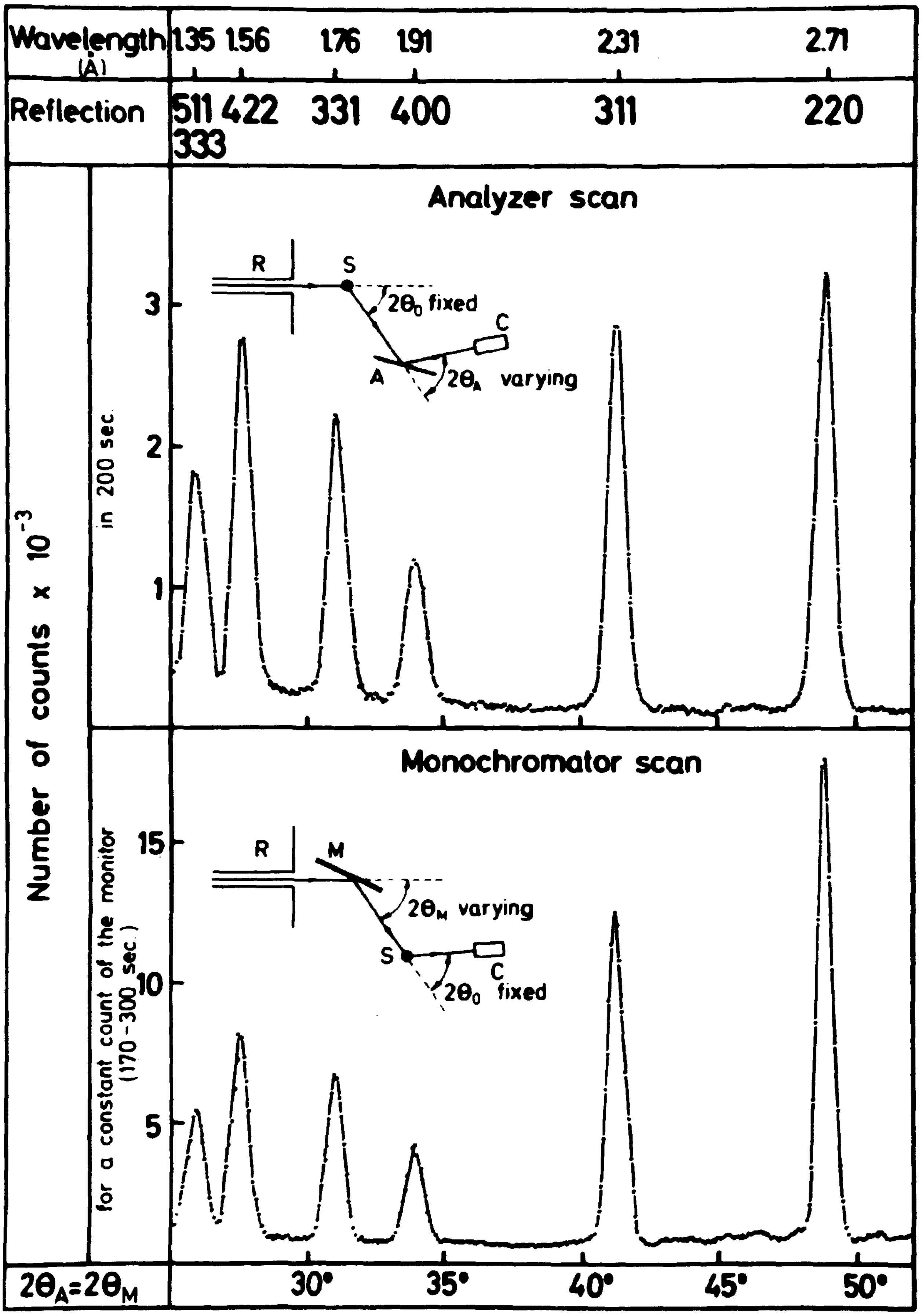

Fig. 10. Neutron diffraction patterns of powdered silicon (90° scattering angle) obtained by the analyser scan method (upper figure) and the monochromator scan method (lower figure). R-reactor, S-sample, M-single crystal monochromator, A-single crystal analyser, C-counter.

Neutron Diffraction by Moving Crystals

(B. Buras, J. K. Kjems, and K. Carneiro)

It has been suggested[1] that a moving single crystal might serve both as a slow-neutron wavelength analyser of special features and as a neutron slowing-down device. These applications have now been demonstrated experimentally.

In both cases the crystal (mounted on a rotating wheel) was moving with a velocity of h/2md (h - Planck's constant, m - neutron mass, d - interplanar spacing) perpendicularly to the diffracting plane. For the mica crystals (d = 10 Å) used in the experiment this velocity was about 200 m/s.

In the analysing case[2] the neutron beam to be analysed is parallel to the reflecting plane and neutrons of different wavelengths are simultaneously reflected through different reflection angles and recorded by a position-sensitive detector connected to a multichannel pulse height analyser. Fig. 11 shows the result of such an analysis of a neutron beam obtained by Bragg reflection of a "white" neutron beam from a pyrolytic graphite monochromator set in a position to give neutrons of wavelength 4.06 Å from the (002) reflection. In addition to this first-order reflection the second, third, and fourth-order reflections are clearly visible.

The main advantages of that type of analyser are the following:

(a) The whole spectrum is recorded in one run in contrast to a non-moving single crystal analyser which records one wavelength at a time.

(b) Higher-order contaminations do not exist.

(c) No long wavelength limit exists for the moving crystal analyser in contrast to non-moving single crystal analysers which can be used only for wavelengths smaller than the Bragg cut-off.

The moving crystal acts as a neutron slowing-down device when in the laboratory frame the incidence angle θ_i of neutrons of wavelength λ_i equals arcsin (λ_i/d) and when, moreover, the crystal moves with the velocity h/2md in the direction of the incident neutron wavevector component normal to the reflecting plane. In this way (with the same experimental set-up as in the analysing case) neutrons of wavelength 17.1 Å were obtained from 8.6 Å neutrons, see fig. 12. Preliminary intensity measurements (taking into account the solid angle and the spread of wavelength) suggest that such a device might be useful for obtaining long neutron wavelengths.

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1) B. Buras and T. Giebultowicz, Acta Cryst., A 28, (1972) 151-153.

2) B. Buras and J. K. Kjems, Nucl. Instr. and Meth. (in print).

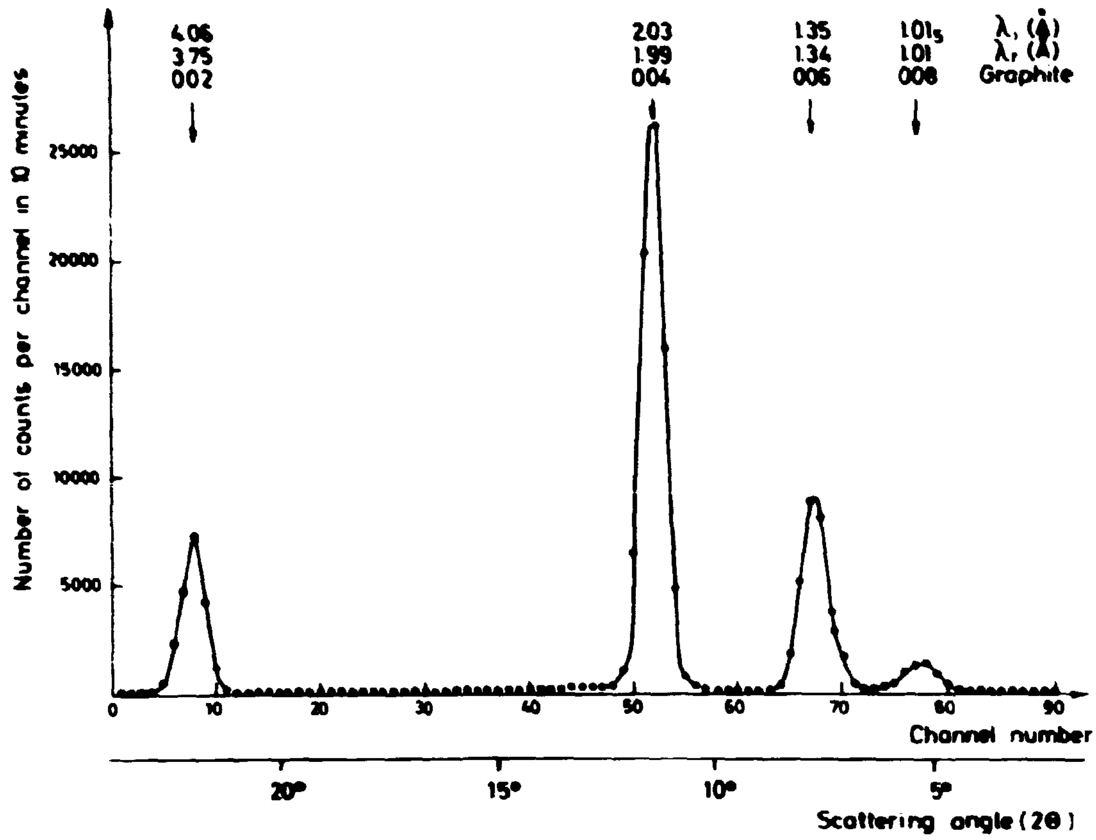

Fig. 11. The spectrum (measured by means of a moving single crystal and a position-sensitive detector connected to a multichannel pulse height analyser) of a neutron beam obtained by Bragg reflection of a polychromatic beam from a pyrolytic graphite monochromator set in a position to give neutrons of wavelength 4.06 Å from the (002) reflection. λ_i-incident neutron wavelength, λ_r-reflected neutron wavelength.

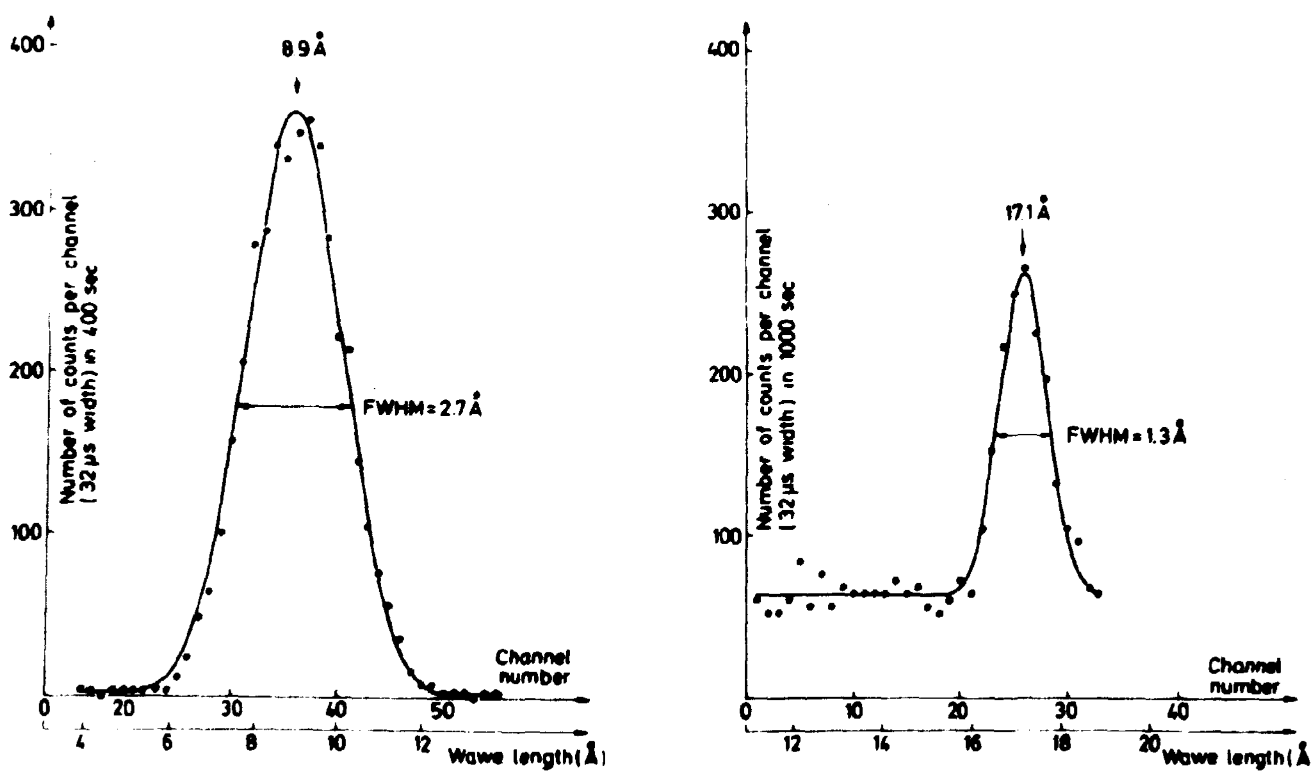

Fig. 12. The time-of-flight spectrum of 8.6 Å neutrons reflected by a mica crystal moving with a velocity of (a) 18.4 m/s and (b) 196 m/s.

Growth of Crystals of the Rare Earth Metal

(K. A. McEwen, P. Touborg (Technical University of Denmark))

Three techniques have been developed to produce single crystals of the rare earth metals and alloys for neutron scattering and magnetization experiments. The strain-anneal method has been employed for Sm and the heavy rare earth metals Gd and Tm. Pr, Nd, Eu, and PrNd crystals have been made by Czochralski pulling from the melt contained in a water-cooled crucible. Impurities in the materials often inhibit crystal growth. Purification of the metals is being pursued by distillation (Eu) and float zone melting techniques (Pr) to achieve larger crystals suitable for precision inelastic neutron scattering experiments.

2. PLASMA PHYSICS

Magnetically Driven Shock Experiment

(C. T. Chang)

The electron temperature, T_e, in the shock experiment was determined from the relative intensities of the He II-4686 and He I-5876 lines[1,2]. T_e, averaged over a 1 μsec time interval,is around 4 eV for a pressure range of 0.2 to 0.5 torrs at a discharge voltage of 13 kV, being slightly higher at the lower pressure. However, owing to the uncertainty of the opacity around $\lambda = 303$ Å (the He II-L_α resonance line), the uncertainty in T_e is $\pm$ 0.5 eV. The average electron density, n_e, as determined from the half width[1] of the above lines is around 10^{17} cm^{-3} and is only slightly dependent on the discharge pressure. The value agrees well with a previous estimate from differential interferograms. The available test time (time elapsed between the arrivals of the shock front and the current sheet respectively, at a fixed axial position) was measured with a piezo-electric pressure probe and a magnetic probe with the He I-5876 line as an intermediary. The results were checked with differential interferograms. The general tendency of the results is: a longer test time for a slower current sheet and for a longer travel of the sheet provided that the second discharge is not initiated. The measured values are considerably lower than the calculated ones based on the conservation of mass and the effect of ionization. Theoretical considerations indicate that the extremely short test time could be due to a leaking current sheet caused by inefficient ionization and/or a charge transfer mechanism.

Solid - Plasma Interaction

(C. T. Chang, A. H. Sillesen, H. Sørensen, and F. Øster)

Refuelling of future fusion reactors by means of frozen pellets injected with a high velocity is a much discussed possibility. The method is feasible only if the pellets are screened from the fusion plasma. Theoretically two different shielding mechanisms may exist, one electrostatic and one magnetic. In a fusion reactor the electron and ion temperatures are likely to be comparable. Therefore both the particle and energy fluxes on the pellet

1) H. R. Griem, Plasma Spectroscopy (McGraw-Hill, 1964).

2) R. Mewe, Brit. J. Appl. Phys. 18, 107 (1967).

will be predominantly from electrons. Thus the pellet may become negatively charged and the subsequent electrostatical shielding will diminish the energy input. Another shielding effect arises if the kinetic pressure of the so-called balloon plasma (the plasma formed by ionization of the sublimed molecules from the pellet) exceeds the magnetic field pressure (magnetic shielding). If either of these two mechanisms operates with sufficient efficiency, the pellet scheme is promising.

We reconsidered the magnetic shielding model, taking into account the latest fusion reactor parameters envisaged, namely the temperature $kT = 20$ keV, the density $n = 2 \times 10^{14}$ cm^{-3}, and the ratio between the kinetic and the magnetic pressure $\beta = 0.03$. Theory predicts that for a pellet of radius between 1 and 10 mm, the lifetime will not be increased considerably. Only at higher β-values will the balloon form.

Other theoretical studies have been started, aiming at estimating the relative importance for the pellet-refuelling problem of specific physical processes, such as aerodynamic ablation during the pellet entry into the reactor, heat transfer involving phase changes during the early phase, possible cracking and disintegration owing to thermal stress.

A preliminary calculation of the aerodynamic heating was compared with the electron energy flux for different plasmas. These calculations show that for plasma parameters of a typical fusion reactor proposal (Rose[1)]), the aerodynamic heating is the lower by three orders of magnitude. For a plasma experiment like the Zeta, however, the two heatings are comparable.

Experimentally, interaction studies between 1/4 mm solid hydrogen pellets and the rotating plasma in the puffatron were continued. The radial interaction position and the angle between the launching direction and the $\bar{E} \times \bar{B}$ direction was varied. After the interaction the pellet is collected and the remaining mass is measured. To determine the exact interaction position and to observe the interaction visually, image converter pictures were taken, looking along the axis of the machine.

The ion energy in the rotating plasma colliding with the pellet was varied from 100 eV up to 1 keV. No clear relationship between the plasma energy and the measured pellet loss was found. The loss itself is one order of magnitude higher than expected on the basis of the theoretical models. A possible reason for the high ablation rate observed might be that the cold,

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1) Rose, D.I. Culham Laboratory Technology Division Memorandum No. 82 (1968).

neutral gas layer formed around the pellet by sublimation is destroyed by the charge-exchange process

$$H^+ + H_2 \rightarrow H + H_2^+ .$$

This process transfers the charge from an energetic ion to a cold neutral, which is consequently accelerated by the crossed $\bar{E}$ and $\bar{B}$ fields, thus removing the protective layer around the pellet. To study the importance of this process in the interaction, the loss will be measured in a helium plasma also. The loss should turn out to be considerably less for helium.

The interaction forms a tail behind the pellet in the $\bar{E} \times \bar{B}$ direction. The light in the tail might come from excited neutrals formed by dissociation of the H_2^+ ions from the charge-exchange processes. The length of the tail fits reasonably well with estimates based on the dissociation cross sections assuming an electron energy of 20 eV.

We are trying to obtain high spatial resolution in holographic interferometry. This will hopefully allow us to diagnose the interaction zone very close to the pellet.

The interaction between a fusion plasma and a solid hydrogen pellet is actually a complex sum of many different interactions. It is therefore planned to study some of these basic interactions in a set-up where a surface of solid deuterium is bombarded by beams of particles with energies up in the keV range. A first version of a set-up for producing solid deuterium films was tested, and based on the experience gained a second version is being built. The film is produced when a molecular beam of deuterium impinges on a quartz crystal kept at 4.2 K. The deuterium solidifies on the quartz crystal, which acts as a microweight. Film thicknesses up to 20 μm were obtained.

Rotating Plasma Experiment (Puffatron)

(A. H. Sillesen, Bjørn Bonnevier (guest from K. T. H., Stockholm))

An attempt was made to investigate fast breakdown phenomena in an $\bar{E} \times \bar{B}$ field configuration. Especially in the case of deuterium lack of reproducibility made the experiments difficult. Three different modes of breakdown were observed. The work has not yet been finished.

Quiescent Plasmas

(G. B. Christoffersen, N. D'Angelo, V. O. Jensen, P. Michelsen, H. L. Pecseli, P. I. Petersen, and L. P. Prahm)

The experimental work at the Q-machine was concentrated on the propagation of perturbations of the plasma in the ion acoustic regime. The conclusion of this work is that the propagation is mainly governed by free streaming ions as long as the electron temperature is lower than or comparable to the ion temperature ($Te/Ti < 5$). In other words, collective interactions are negligible in this case. Weak shock measurements led to the same conclusion.

To study the importance of collective interactions it is therefore necessary to increase the electron temperature, and several methods were tried out. The preliminary results show that it is possible to increase the electron temperature by a factor of 4-6. Theoretically the linearized Vlasov equation for the ions was solved as a boundary-value problem. Normally the Vlasov equation is solved by applying the "first pole approximation". A comparison of our solutions and the usual approximated ones shows that the "first pole approximation" is incorrect. Especially it is shown that an exponentially damped wave, which is always obtained in a "first pole approximation", is not a mathematically possible solution to the Vlasov Equation.

The propagation of weak whocks was studied theoretically by means of the Green function techniques. The calculations show that the collective interactions are negligible in an ordinary Q-machine plasma as verified by the conclusions from the experiments mentioned above.

An investigation of microinstabilities in a magnetizied plasma was started. It is believed that a more exact calculation based on the Green function method will give results which differ considerably from those obtained earlier.

3. METEOROLOGY

Velocity Profiles

(E. L. Petersen and P. A. Taylor (University of Southampton, England))

Analyses of data from Risø's 120 m tower show that for certain wind directions distinct kinks appear in the vertical wind profiles of the horizontal mean wind. The kinks relate to changes in the roughness of the upstream terrain surface and have been discussed within the framework of the Monin - Oboukhov theory.

The measured profiles were compared with the predictions by numerical models for boundary layer flow over an abrupt change in terrain roughness. The agreement between the data and the models is moderately good. The deviations resulted in refinements of the models, especially by taking into account also the change of terrain level across the coastline of the Risø peninsula.

Meso-Scale Effects in the Tower Data

(W. Klug (Technishe Hochschule, Darmstadt) and E. L. Petersen)

A number of distinct features, possibly of meso-scale origin, were detected in the tower data. For example it was found that the horizontal wind vector shows a remarkable turning with height, a turning consistently depending on the time of the day and the year. In order to explain these features, a numerical model was planned and partly established. The primary intention is to study the influence of the daily heating of a thermally inhomogeneous surface on the spatial structure of the mean flow. The results look promising, but it is too early to draw final conclusions.

Spectral Analysis of Climatological Data

(E. L. Petersen)

The spectral analyses of wind and temperature data from the Risø tower were completed. It was shown that a physically relevant representation of the horizontal velocity spectra should be based upon spectra of the components of the wind vector along two perpendicular directions and not on the wind speed spectra.

Analysis of the Greenland Ice Data

(S. E. Larsen and E. L. Petersen)

From an ice core from Camp Century in Greenland samples were obtained of the precipitation in Greenland during the last 130 000 years. By measurements of the ratio between the oxygen isotopes 0^{18} and 0^{16}, it is possible to estimate the temperature at which the water vapour condensed.

The variations in the ratio between the isotopic abundances of 0^{16} and 0^{18} in the ice are currently being analysed by the Geophysical Isotope Laboratory at the University of Copenhagen. Since the analysis of the full sample series is a lengthy affair, it was decided to start the statistical analysis on a short segment of the total series (1174-1966 AD). This analysis was started by the Geophysical Isotope Laboratory and was later completed in co-operation with the Meteorology Section at Risø.

The purpose of this analysis was partly to test the various statistical methods to be used on the entire record later on, partly to see how the ice data compared with other temperature records from the recent past.

From the analysis, the following tentative results may be extracted. There seems to be statistical significance for long time periodicities in the record. However, this must be studied in more detail when longer segments of the total record can be included in the analysis.

Various statistical prediction methods all predict that the last fifty years of this century will be colder than the first. There is excellent agreement between the last 200 years of the ice data and temperature records in Europe and North America.

In fig. 13 the ice data are used as the low-frequency part of the composite temperature spectrum. The $0^{18}/0^{16}$ ratio was scaled using a 186-year temperature series from Hohenpeissenberg in southern Germany.

Climatology in Greenland

(N. E. Busch, L. Kristensen, and J. Taagholt)

The governmental decision to close the Danish airport Nord in North East Greenland by the end of June 1972 meant that the meteorological and other geophysical observations could not be continued.

At the spring meeting in 1972 of the Commission for Scientific Investigation in Greenland, the director of the Danish Meteorological Institute was urged to establish an automatic climatological station at Nord in order to continue the almost twenty-year-old climatological record. Based on a

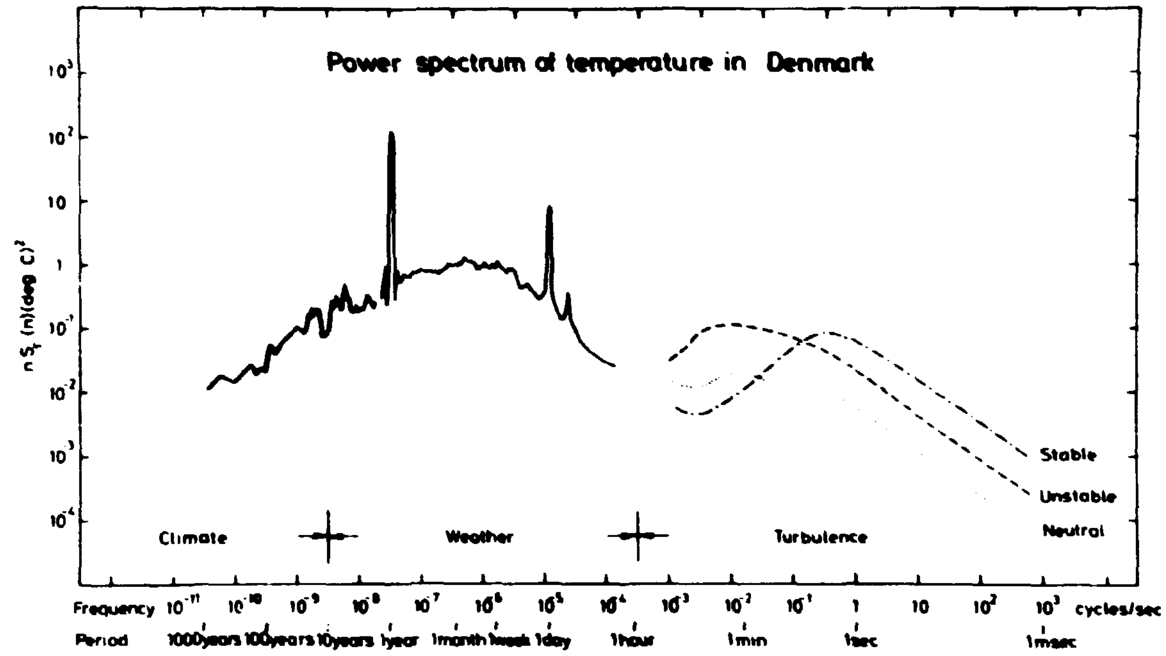

Fig. 13. Composite power spectrum of the temperature. ▬▬: Yearly averages of the O^{18}/O^{16} ratio in precipitation from 1174 to 1966. The data are taken from an ice core from Greenland and calibrated against a two-hundred-year temperature record from Southern Germany. ——: Hourly temperature measurements, averaged over ten minutes, taken at Risø, 1958-1967 ----, ····· and -·-·-·: Temperature data measured in Kansas in 1968 for three different cases of atmospheric stability (Z/L = -0.5, -0.03, and 0.5).

recommendation from a number of scientists (geographers, glacialogists, climatologists, zoologists, and botanists), a working group started to investigate the possibility of installing an Unmanned Geophysical Observatory (UGO) at Nord. Although a request for financial support of this project was not met, the meteorology section at Risø and staff members from different departments of the Meteorological Institute continued their efforts, which resulted in the installation of a simple climatological station. The UGO-NORD records air temperature, pressure, wind speed, and wind direction once every hour. These data are recorded by means of a small transportable datalogger equipped with a magnetic-tape recorder.

The installation took place in the beginning of June 1972 with only one month of preparation (see fig. 14). Although the system is designed to operate for one year without inspection and maintenance, an opportunity to replace the datalogger with another one and thereby check the performance was taken when the Royal Danish Air Force paid Nord a short visit in August. The data recorded so far show that UGO-NORD operates satisfactorily.

As long as Nord remains unmanned, it is doubtful whether the station will and can be reached by air. However, co-operation with the sledge

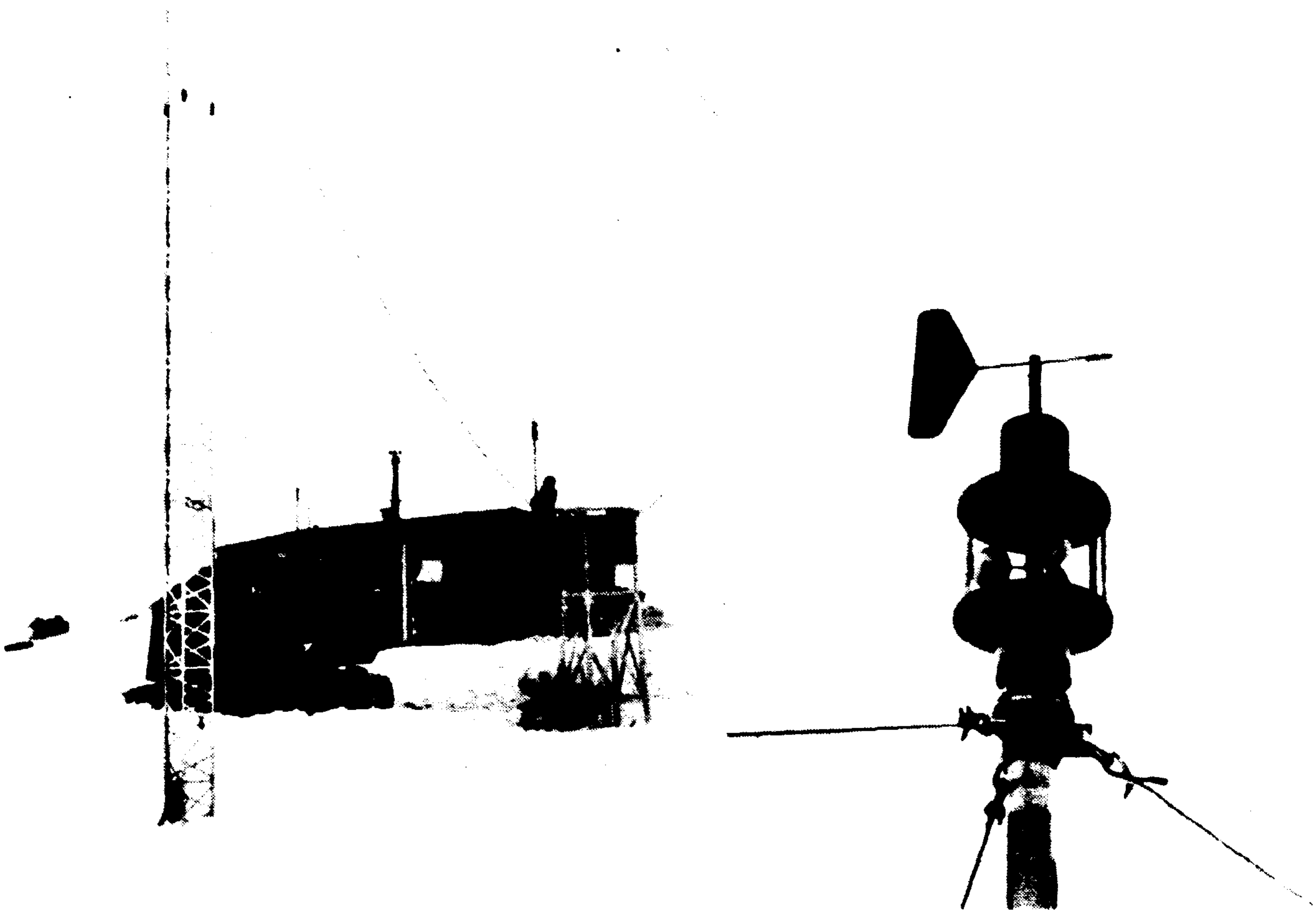

Fig. 14. The automatic climatological station UGO-NORD at Nord in North-Eastern Greenland. To the left the telestation and its surroundings. To the right a close-up of the cup anemometer and the wind vane which are mounted 5.33 metres above the ground on top of a steel pipe.

patrol "SIRIUS" ensures that UGO-NORD will be checked and the recorded data recovered whenever the sledge patrol visits the area.

<u>Air - Sea Interaction</u>

(N. E. Busch, L. Kristensen, and S. E. Larsen)

Information about the interaction between sea and atmosphere is important for the understanding of the development of the weather on any scale. It is in this connection of interest to measure turbulent fluxes of heat, water vapour, and momentum as well as mean wind profiles and mean temperature profiles close to the sea surface. However, such experiment are difficult because of the need for a stable platform for the instruments on the open sea.

In the spring of 1972 the meteorology section in co-operation with oceanographers from the Geophysical Institute of the University of Bergen and from the Institute for Physical Oceanography of the University of Copenhagen carried out a pilot experiment with the purpose of testing the techniques involved in raising and instrumenting a 40-metre-high tower on 25 metres of water near Store Middelgrund in Kattegat (position $56^{0}36'$N, $12^{0}05'$E) (see fig. 15).

Fig. 15. The air - sea interaction experiment "Kattegat 72". Raising of the tower. The Risø cutter "Fyrholm" participated in the experiment.

The part of the tower under water was to carry instruments for measuring current-, salinity-, and temperature-profiles, water level, internal waves, and optical parameters.

Instruments for simultaneous measurements of wind speed profiles, wind direction, and temperature profiles were to be mounted on the part of the tower over the sea surface.

Owing to the rough weather conditions during the experiment there was time only for raising the tower. In order not to lose instruments during installation, instrumentation for wind and air tem erature measurements was not mounted.

Because of the difficulties experienced with the erection of a tower on deep water, it was decided that some changes in the design of the tower were needed. The meteorology section undertook the task of conducting these modifications.

According to the plans an oceanographical-meteorological experiment "Kattegat 73" using such a tower will take place in the spring of 1973.

Applied Meteorology

(N. E. Busch, L. Kristensen, S. E. Larsen, and E. L. Petersen)

This year, as earlier, the meteorology section undertook a number of tasks of an applied nature. Among these were: site evaluation and dispersion modelling, development and testing of meteorological instruments, air pollution studies, and evaluation of dynamic effects of wind on buildings and other structures.

Development of Meteorological Instruments

It has been demonstrated that in order to exploit more refined hot-wire configurations for anemometry, it is necessary to mount the probes on a fast-responding wind vane. The development and testing of such an instrument carrier is now being completed at Risø. In the future, it will be manufactured by DISA Electronics.

The cup anemometers "Risø 70", developed at Risø in co-operation with the firm of G. Schultz, will now be supplied with new light-weight cup assemblies made of carbon-reinforced plastic. A collaboration between the meteorology section and the Metallurgy and the Chemistry Departments resulted in the development of a production scheme for this extremely strong material, which consists of randomly oriented, 10-mm long carbon fibres dispersed in a matrix of Araldite (cr 230).

4. LIQUID-N_2 AND -He PLANTS

The production of liquid N_2 and He amounted to 141000 and 14000 litres respectively. Out of these, 5000 litres of liquid He was delivered to laboratories in Copenhagen and Århus.

5. EDUCATIONAL ACTIVITIES AND PUBLICATIONS

Lectures

J. Als-Nielsen, Nuclear Physics (50 lectures). Technical University of Denmark.

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1) Bell Telephone Laboratory, N.J. USA (June 1972).
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2) University of Sheffield, England (February 1972).
3) University of Birmingham, England (February 1972).
4) University of Edinburgh, Scotland (February 1972).
5) University of Reading, England (February 1972).
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Degrees, Students, etc.

During the period the following members of the staff acquired the following degrees:

G. Christoffersen	lic. techn.
Jens Jensen	lic. techn.
P. A. Reynolds	(Ph. D. - Oxford).

The following postgraduate students carried out research at the Physics Department leading to the degree of lic. techn. or Ph. D.:

Per Bak	(Solid-State Physics)
Kim Carneiro	(Solid-State Physics)
Oluf Danielsen	(Solid-State Physics)
Niels Otto Jensen	(Meteorology)
Hans Pecseli	(Plasma Physics)
E. Lundtang Petersen	(Meteorology)
Peter I. Petersen	(Plasma Physics)
Jack Wenzel	(Solid-State Physics)

The following undergraduates of Danish universities completed or is working on master's thesis projects at the department:

Leif Wagner Jørgensen	(Plasma Physics)
Niels Woetman Nielsen	(Meteorology)
Ole Rathmann	(Solid-State Physics)

Four foreign students sponsored by the IASTE carried out practical work at the department as part of their general training.

6. STAFF OF THE PHYSICS DEPARTMENT

Hans Bjerrum Møller (head of department)

G. Stauning
(office staff)
A. Frellsen

1. Solid-State Physics (Neutron Physics)

University Graduates

Jens Als-Nielsen

O. Krogh Andersen (Consultant, Technical University of Denmark)

Per Bak (Ph. D. -student)

B. Buras (also at the H. C. Ørsted Institute)

Kim Carneiro (Ph. D. -student)

Oluf Danielsen (Ph. D. -student)

Ove W. Dietrich

Jens Gylden Houmann

Lewis Holmes (also at the Technical University of Denmark)

Jens Jensen

K. Krejov (IAEA stipendiate)

Jørgen Kjems (at Brookhaven National Laboratory from September)

C. U. Linderstrøm-Lang (Chemistry Department)

Bente Lebech

Per-Anker Lindgård (at Bell Laboratories until 18 October)

K. A. McEwen (Also at the H. C. Ørsted Institute)

Hans Bjerrum Møller

Mourits Nielsen (at Oak Ridge National Laboratory from September)

B. M. Powell

P. A. Reynolds (until 21 December)

Elisabeth Warming (at the University of Cambridge until 15 May)

Jack Wenzel (Ph. D. -student).

Technicians

Bjarne Breiting

Kaj Christensen

S. E. Christensen (until 30 November)

Arent Hansen

B. Heiden

John Z. Jensen

Louis G. Jensen

Steen Jørgensen

W. Kofoed

J. Linderholm

A. Thuesen

2. Plasma Physics

University Graduates

C. T. Chang

G. Christoffersen (until 31 August)

N. D'Angelo (consultant, Dansk Rumforskningsinstitut)

Vagn O. Jensen

Poul Michelsen (at Yale University)

Hans Pecseli (Ph. D. -student)

Peter I. Petersen (Ph. D. -student)

L. Prahm (Ph. D. -student) (until 31 July)

A. H. Sillesen

Hans Sørensen

Flemming Øster

Technicians

Bendix Bordrup

B. Hurup Hansen

Mogens Nielsen

Arne Nordskov

John Petersen

Børge Reher

Jane Doyle (temporary assistant)

3. Nuclear Physics

University Graduates

Verner Andersen

Carl Jørgen Christensen

Technicians

Poul Andersen

Finn Hansen

4. Meteorology

University Graduates

Niels E. Busch

John A. Dutton (visiting scientist August-71 - August-72)

Niels Otto Jensen (Ph. D. -student)

Leif Kristensen

Søren Larsen

N. Woetmann Nielsen (Masters thesis project-student)

E. Lundtang Petersen (Ph. D. -student)

Technicians

Jørgen Christensen

Gunner Dalsgård

Morten Frederiksen

Gunnar Jensen

Knud Sørensen

5. Liquid-N_2 and -He Plant

Technicians

John Z. Jensen

Sv. E. Christensen (until 30 November)

The following guest scientists spent several months at the department:

B. Bonnevier, KTH, Stockholm	(Plasma Physics)
Victor S. Emery, NORDITA	(Solid-State Physics)
Nigel Hall, Oxford University	(" " ")
K. Hennig, Dubna	(" " ")
Heinz Heer, Würenlingen	(" " ")
Jan Herbst, HCØ (Cornell Univ.)	(" " ")
H.C.S. Hsuan, Univ. of Iowa	(Plasma Physics)
Werner Klug, Darmstadt	(Meteorology)
J.P. McTague, Univ. of Calif.	(Solid-State Physics)
L. Passell, Brookhaven Nat. Lab.	(" " ")
G. Stuart Pawley, Univ. of Edinburgh	(" " ")
H.-G. Purwins, Univ. de Geneve	(" " ")
B.D. Rainford, Imperial College	(" " ")
R. Rinaldi, Univ. of Edinburgh	(" " ")
G. Shirane, Brookhaven Nat. Lab.	(" " ")
R. Stedmann, AB Atomenergi	(" " ")

P. A. Taylor, Univ. of Southampton	**(Meteorology)**
John Twisleton, Oxford University	**(Solid State Physics)**
J. W. White, Oxford University	**(" " ")**
J. W. Wilkins, HCØ (Cornell Univ.)	**(" " ")**